Agroscope Science | No. 194 / 2024

Process-oriented modeling of direct N_2O emissions from agricultural soils

Project LACHSIM

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Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
Agroscope

Agroscope good food, healthy environment

Imprint

Publisher	Agroscope Reckenholzstrasse 191 8046 Zurich www.agroscope.ch
Information	marcio.dosreismartins@agroscope.admin.ch
Cover Photo	Carole Parodi, Agroscope
Download	www.agroscope.ch/science
Copyright	© Agroscope 2024
ISSN	2296-729X
DOI	https://doi.org/10.34776/as194e

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Abbreviations

AF	alfalfa (*Medicago sativa* L.)
APSIM	Agricultural Production Systems Simulator
BD	bulk density
biomax	biomass above which DayCent parameters pramn(1,2) and pramx(1,2) are equal, respectively, the minimum and maximum C:N ratios of the new growth
BIOORG	organic farming treatment with manure and slurry as N fertilization
BNF	biological N_2 fixation
CC	catch or cover crop
CH_4	methane
CL	clover (*Trifolium* spp.)
CO_2	carbon dioxide
CONFYM	conventional farming treatment with manure plus additional mineral fertilization
CONMIN	conventional farming treatment with only mineral fertilization
cr	cover crushing
DayCent	Daily CENTURY Model
DNDC	Denitrification-decomposition Model
ecosys	Comprehensive Model of Natural and Managed Ecosystems
EF	emission factor
EPIC	Environment Policy Integrated Climate Model
ETH	Federal Institute of Technology (Eidgenössische Technische Hochschule)
F	synthetic fertilizer
FB	faba bean (*Vicia faba* L.)
FOAG	Federal Office of Agriculture (Bundesamt für Landwirtschaft / Office fédéral de l'agriculture)
FOEN	Federal office for the environment (Bundesamt für Umwelt / Office fédéral de l'environnement)
FSO	Federal Statistical Office (Bundesamt für Statistik / Office fédéral de la statistique)
GC	grass-clover ley
GHG	greenhouse gas
GM	green manure
GWP	global warming potential
hb	herbicide
IDAweb	Data Portal for Teaching and Research of MeteoSwiss
IPCC	Intergovernmental Panel on Climate Change

KOBO	National Competence Center for Soil (Kompetenzzentrum Boden/ Centre de compétences sur les sols)
K_{sat}	saturated hydraulic conductivity
LOO	leave-one-out
LULUCF	land use, land-use change and forestry
M	manure
MAP	mean annual precipitation
MAT	mean annual temperature
MeteoSwiss	Federal Office of Meteorology and Climatology (Bundesamt für Meteorologie und Klimatologie/Office fédéral de météorologie et de climatologie)
mod	modeled value
$\overline{mod}$	average of modeled values
MU	mustard (*Sinapis alba* L.),
MZ	maize (*Zea mays* L.),
N_2	dinitrogen
N2N2Oadj	N_2:N_2O ratio adjustment coefficient
N_2O	nitrous oxide
N2Oadjust_fc	maximum proportion of nitrified N lost as N_2O at field capacity
N2Oadjust_wp	minimum proportion of nitrified N lost as N_2O at wilting point
Ncoeff	minimum water and temperature limitation coefficient for nitrification
netmn_to_no3	fraction of new net mineralization that goes to NO_3^-
NFI	National forest inventory (Landesforstinventar / inventaire forestier national)
NH_4^+	ammonium
NO	nitric oxide
NOFERT	unfertilized control treatment
OA	oat (*Avena sativa* L.)
obs	observed value
$\overline{obs}$	average of observed values
PaSim	Pasture Simulation Model
PE	peas (*Pisum sativum* L.)
PEST	Model-Independent Parameter Estimation
pl	moldboard plowing
PO	potato (*Solanum tuberosum* L.)
ppdf(1)	optimum temperature for growth
pramn(1,1)	minimum aboveground C:N ratio in the beginning of the growth curve
pramn(1,2)	minimum aboveground C:N ratio with biomass > biomax

pramx(1,1)	maximum aboveground C:N ratio in the beginning of the growth curve
pramx(1,2)	maximum aboveground C:N ratio with biomass > biomax
prdx(1)	coefficient for calculating potential production as a function of solar radiation
PTF	pedotransfer function
Q_1	first quartile of the observed values
Q_3	third quartile of the observed values
QCLAS	quantum-cascade laser absorption spectrometer
R^2	coefficient of determination
RMSE	root mean square error
rl	rolling
RP	rapeseed (*Brassica napus* L.)
RPIQ	ratio of performance to interquartile distance
rRMSE	relative root mean square error
RY	rye (*Secale cereale* L.)
S	slurry
S1	reference system treatment
S2	no-tillage system treatment
S3	integrated weed management system treatment
S5	fully integrated weed management system treatment
SB	summer barley (*Hordeum vulgare* L.)
SF	sunflower (*Helianthus annuus* L.)
snfxmx(1)	maximum BNF rates
SOC	soil organic carbon
SP	spelt (*Triticum spelta* L.)
st	shallow tillage
SY	soybeans (*Glycine max* (L.) Merr)
TERENO	Terrestrial Environmental Observatories
Tier1	first level of methodological complexity for calculating GHG emissions defined by IPCC (lowest complexity)
Tier3	third level of methodological complexity for calculating GHG emissions defined by IPCC (highest complexity)
TR	triticale (*Triticale hexaploide* Lart.)
UNFCCC	United Nations Framework Convention on Climate Change
WB	winter barley
WFPS	water-filled pore space
wfpsdnitadj	adjustment on inflection point for WFPS effect on denitrification

WSL	Federal Institute for Forest, Snow and Landscape Research (Eidgenössische Forschungsanstalt für Wald, Schnee und Landschaft/ Institut fédéral de recherches sur la forêt, la neige et le paysage
WW	winter wheat (*T. aestivum* L.)

Summary

Under the United Nations Framework Convention on Climate Change (UNFCCC), industrialised countries and countries with economies in transition (the so-called Annex 1 countries) are encouraged to move towards more sophisticated approaches for national greenhouse gas reporting. Developing a model-based approach for estimating nitrous oxide (N_2O) emissions from agricultural soils encompasses crucial steps of sound model selection, calibration, evaluation and upscaling of the model simulations to the regional level. To implement a model-based approach to simulate N_2O emissions from agricultural soils in Switzerland, we selected the biogeochemical model DayCent considering its level of complexity and the availability of inputs required for regional simulations of N_2O emissions. In the second step, we used extensive daily N_2O flux observations from six cropland sites (four in Switzerland and two in France) and four grassland sites (two in Switzerland and two in Germany) to conduct automatic data-driven calibration of DayCent. After site-specific calibration, a leave-one-out (LOO) cross-evaluation was conducted for each land use type (*i.e.* cropland and permanent grassland) to assess the ability of the model to predict N_2O emissions for sites it was not calibrated for. The LOO cross-evaluation resulted in an R^2 of 0.63 for the prediction of N_2O emissions from croplands and 0.65 from grasslands, compared to R^2 values of 0.51 and 0.45 obtained with default parameterisation for croplands and grasslands, respectively. Overall, our results showed that the improvement in N_2O predictions was usually associated with the adjustment of only a few 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). For grasslands, in addition to these parameters controlling N transformation in the soil, the adjustment of parameters related to N uptake by plants (thresholds of N sufficiency and deficiency and maximum biological N_2 fixation) also affected the model's ability to predict N_2O emissions. These parameters also affected the simulation of N leaching, which is an indirect source of N_2O. Overall, model-based estimates of N_2O emissions were clearly closer to measurements than estimates based on commonly used emission factor (EF) approaches for both croplands and grasslands. Our results showed that, after data-driven calibration of only a few N cycle parameters in soil and plants, DayCent simulations are useful for reporting N_2O emissions from agricultural soils in Switzerland. Therefore, in the last phase of the project, we performed a first upscaling of DayCent simulations of soil N_2O emissions to the national level. For the upscaling, we gathered and processed geospatial data on of land use, soil properties, and weather variables at the country scale. In this preliminary model-based national simulation of N_2O emissions, we stratified the territory and assumed an oversimplification of management practices. Nevertheless, the results of this project indicate that DayCent is an adequate model for reporting N_2O emissions from agricultural soils in Switzerland. Obtaining more accurate management data is a crucial, necessary step towards establishing model-based estimates of N_2O emissions for the national greenhouse gas inventory.

Zusammenfassung

Im Kontext der Klimarahmenkonvention der Vereinten Nationen (UNFCCC) werden Industrieländer und Länder mit Transformationsökonomien (sogenannte Annex-1-Länder) dazu aufgefordert, komplexere Ansätze für die nationale Berichterstattung von Treibhausgasemissionen zu übernehmen, beispielsweise mithilfe von Modellen. Hierzu sind Modellauswahl, Kalibrierung, Auswertung und Hochskalierung der Simulationen auf die regionale Skala grundlegende Schritte. Zur Implementierung eines modellbasierten Ansatzes zur Simulation von Lachgasemissionen (N_2O) aus landwirtschaftlichen Böden in der Schweiz haben wir uns aufgrund seiner Komplexität und der Verfügbarkeit der für regionale Simulationen von N_2O-Emissionen erforderlichen Eingangsdaten für das biogeochemische Modell DayCent entschieden. In einem zweiten Schritt nutzten wir umfangreiche tägliche Messungen der N_2O-Emissionen von sechs Ackerlandstandorten (vier in der Schweiz und zwei in Frankreich) und vier Grünlandstandorten (zwei in der Schweiz und zwei in Deutschland), um eine automatische datengesteuerte Kalibrierung von DayCent durchzuführen. Nach einer standortspezifischen Kalibrierung wurde für jeden Landnutzungstyp (d. h. Ackerland und Dauergrünland) eine «Leave-One-Out-cross evaluation» (LOO) durchgeführt, um die Fähigkeit des Modells zu beurteilen, N_2O-Emissionen für Standorte vorherzusagen, für die es nicht kalibriert wurde. Die LOO-Auswertung ergab einen R^2-Wert von 0.63 für die Vorhersage von N_2O-Emissionen aus Böden auf Ackerland und 0.65 auf Dauergrünland, verglichen mit R^2-Werten von 0.51 und 0.45, die mit der Standardparametrisierung für Ackerland bzw. Dauergrünland erzielt wurden. Insgesamt zeigten unsere Ergebnisse, dass die Verbesserung der N_2O-Vorhersagen normalerweise mit der Anpassung nur einiger weniger Parameter verbunden war, die den Stickstoffkreislauf im Boden steuern (z. B. die maximale tägliche Nitrifikationsmenge und der Wendepunkt für die Auswirkung des wassergefüllten Porenraums auf die Denitrifikation). Bei Dauergrünland beeinflusste neben diesen Parametern, welche die Stickstoffumwandlung im Boden steuern, auch die Anpassung von Parametern im Zusammenhang mit der Stickstoffaufnahme durch Pflanzen (Schwellenwerte für Stickstoffüberschuss und -mangel und maximale biologische N_2-Fixierung) die Fähigkeit des Modells, N_2O-emissionen vorherzusagen. Diese Parameter beeinflussten auch die Simulation der Stickstoffauswaschung, die eine indirekte Quelle von N_2O-Emissionen ist. Insgesamt lagen modellbasierte Schätzungen der N_2O-Emissionen sowohl für Ackerland als auch für Dauergrünland deutlich näher an den beobachteten Werten als Schätzungen, die auf Emissionsfaktoren basieren. Unsere Ergebnisse zeigten, dass DayCent-Simulationen nach datengesteuerter Kalibrierung von nur wenigen Stickstoffkreislaufparametern in Boden und Pflanze für die Berichterstattung der N_2O-Emissionen aus landwirtschaftlichen Böden in der Schweiz nützlich sind. Daher führten wir in der letzten Phase des Projekts eine erste Hochskalierung der DayCent-Simulationen der N_2O-Emissionen auf die nationale Ebene durch. Für die Hochskalierung sammelten und verarbeiteten wir räumliche Daten zur Landnutzung, zu Bodeneigenschaften und Wettervariablen für die ganze Schweiz. Diese vorläufigen, schweizweiten Berechnungen für N_2O-Emissionen werden für 26 Regionen mit ähnlichen Klimabedingungen und Bodeneigenschaften gemacht. Zudem verwenden wir stark vereinfachte Annahmen für die Bewirtschaftung. Die Ergebnisse dieses Projekts zeigen jedoch, dass DayCent ein geeignetes Modell für die Berichterstattung von N_2O-Emissionen aus landwirtschaftlichen Böden in der Schweiz ist. Die Erhebung genauerer Bewirtschaftungsdaten wird ein entscheidender und notwendiger nächster Schritt zur Quantifizierung modellbasierter N_2O-Emissionen für das nationale Treibhausgasinventar sein.

Resumé

Dans le cadre de la Convention-cadre des Nations Unies sur les changements climatiques (CCNUCC), les pays industrialisés et les pays à économie en transition (appelés pays de l'Annexe 1) sont encouragés à adopter des approches plus sophistiquées en matière d'inventaire national des gaz à effet de serre en utilisant par exemple la modélisation. Pour cela, la sélection du modèle, l'étalonnage, l'évaluation et extrapolation des simulations au niveau régional sont des étapes fondamentales. Pour simuler les émissions de protoxyde d'azote (N_2O) des sols agricoles en Suisse, nous avons sélectionné le modèle biogéochimique DayCent compte tenu de son niveau de complexité et de la disponibilité des données d'entrée pour les simulations régionales des émissions de N_2O. Dans un deuxième temps, nous avons utilisé de grands ensembles de données d'observation des flux quotidiens de N_2O sur six sites avec cultures (quatre en Suisse et deux en France) et quatre sites avec prairies (deux en Suisse et deux en Allemagne) pour effectuer un étalonnage automatique de DayCent. Après un étalonnage spécifique au site, une évaluation croisée *leave-one-out* (LOO) a été menée pour chaque type d'utilisation des terres (les cultures et les prairies permanentes) afin d'évaluer la capacité du modèle à prédire les émissions de N_2O pour les sites où il n'était pas étalonné. L'évaluation croisée LOO a abouti à un R^2 de 0,63 pour la prévision des émissions de N_2O des cultures et de 0,65 pour les prairies, contre un R^2 de 0,51 et de 0,45 obtenus avec un paramétrage par défaut respectivement pour les cultures et les prairies. Les résultats ont montré que l'amélioration des prévisions de N_2O était généralement associée à l'ajustement de quelques paramètres contrôlant le cycle de l'azote dans le sol (par exemple, la quantité quotidienne maximale de nitrification et le point d'inflexion de l'effet de l'espace poreux rempli d'eau sur la dénitrification). Pour les prairies, en plus de ces paramètres contrôlant la transformation de l'azote dans le sol, l'ajustement des paramètres liés à l'absorption de l'azote par les plantes (seuils de suffisance et de carence en N et valeur maximale de fixation biologique de N_2) a également affecté la capacité du modèle à prédire les émissions de N_2O. Ces paramètres ont également affecté la simulation de la lixiviation de N, qui est une source indirecte de N_2O. Les estimations des émissions de N_2O basées sur des modèles étaient significativement plus proches des valeurs observées que les estimations basées sur des facteurs d'émission couramment utilisées pour les cultures et les prairies. Les résultats montrent que, avec l'ajustement de seulement quelques paramètres du cycle de l'azote, les simulations avec le modèle DayCent sont utiles pour estimer les émissions de N_2O des sols agricoles en Suisse. Par conséquent, dans la dernière phase du projet, une première mise à l'échelle régionale de la modélisation des émissions de N_2O a été effectuée. Pour cette procédure, nous avons collecté et traité des données géospatiales sur l'utilisation des terres, les propriétés des sols et les variables météorologiques pour les différentes régions de Suisse. Dans cette simulation préliminaire des émissions de N_2O à l'échelle du pays, un découpage du territoire et une approche très simplifiée des pratiques de gestion ont été utilisées. Néanmoins, les résultats de ce projet indiquent que DayCent est un modèle adéquat pour estimer les émissions de N_2O des sols agricoles en Suisse. L'obtention de données de gestion plus précises est une étape cruciale et nécessaire afin d'établir une approche de modélisation des émissions de N_2O pour l'inventaire national des gaz à effet de serre.

Riassunto

La Convenzione quadro sui cambiamenti climatici delle Nazioni Unite (UNFCCC) impegna i Paesi industrializzati e i Paesi ad economia in transizione (cosiddetti Paesi dell'allegato I alla Convenzione) ad adottare approcci più complessi per l'inventario nazionale delle emissioni di gas serra, per esempio sulla base di modelli. La selezione del modello, la calibrazione, la valutazione e l'estrapolazione delle simulazioni su scala regionale rappresentano tappe fondamentali. Per simulare le emissioni di protossido d'azoto (N_2O) dei suoli agricoli in Svizzera abbiamo scelto il modello biogeochimico DayCent in considerazione del suo livello di complessità e della disponibilità dei dati di ingresso necessari per le simulazioni regionali delle emissioni di N_2O. In una seconda fase abbiamo utilizzato vasti insiemi di dati di misurazione delle emissioni quotidiane di N_2O di sei aree coltive (quattro in Svizzera e due in Francia) e quattro aree inerbite (due in Svizzera e due in Germania) per effettuare una calibrazione automatica di DayCent. Dopo una calibrazione specifica per il sito, è stata svolta una validazione incrociata leave-one-out (LOO) per ogni tipo di utilizzo del suolo (ossia superfici coltive e aree permanentemente inerbite) per valutare la capacità del modello di prevedere le emissioni di N_2O nei siti per i quali non è stata effettuata la calibrazione. Dalla validazione incrociata LOO è risultato un valore R^2 di 0,63 per la previsione delle emissioni di N_2O delle superfici coltive e di 0,65 per le aree permanentemente inerbite, rispetto a valori R^2 rispettivamente di 0,51 e 0,45 ottenuti con la parametrizzazione standard per le superfici coltive e quelle prative. Nel complesso i nostri risultati mostrano che il miglioramento delle previsioni per l'N_2O era generalmente associato all'adeguamento di qualche parametro che controlla il ciclo dell'azoto nel suolo (ad es. la quantità massima giornaliera di nitrificazione e il punto di inflessione dell'effetto dello spazio poroso riempito di acqua sulla denitrificazione). Per le superfici coltive, oltre a questi parametri che controllano la trasformazione dell'azoto nel suolo, anche l'aggiustamento dei parametri collegati all'assorbimento dell'azoto da parte delle piante (soglie di sufficienza e di carenza di azoto e valore massimo di fissazione biologica dell'N2) ha influenzato la capacità del modello di prevedere le emissioni di N_2O. Questi parametri hanno influenzato pure la simulazione della liscivazione dell'azoto, che è una fonte indiretta di emissioni di N_2O. Nell'insieme le stime basate su modelli delle emissioni di N_2O erano notevolmente più vicine ai valori osservati rispetto alle stime basate su fattori di emissione normalmente utilizzati per le superfici coltive e quelle prative. I risultati ottenuti dimostrano che, con la calibrazione basata sui dati di pochi parametri del ciclo dell'azoto, le simulazioni con il modello DayCent sono utili per prevedere le emissioni di N_2O nei suoli agricoli in Svizzera. Nell'ultimo stadio del progetto abbiamo quindi proceduto a una prima estrapolazione a livello nazionale delle simulazioni delle emissioni di N_2O effettuate con il modello DayCent. Per questa procedura abbiamo raccolto e trattato dati geospaziali sull'utilizzo dei suoli, le proprietà dei suoli e le variabili meteorologiche per tutta la Svizzera. In questa simulazione preliminare a livello nazionale delle emissioni di N_2O abbiamo utilizzato una stratificazione del territorio e un approccio molto semplificato delle pratiche di gestione. I risultati del progetto dimostrano tuttavia che DayCent è un modello adeguato per l'inventario delle emissioni di N_2O dei suoli agricoli in Svizzera. La rilevazione di dati di gestione più precisi è una prossima tappa fondamentale e necessaria per quantificare le emissioni di N_2O sulla base di modelli per l'inventario nazionale dei gas serra.

1 Aims of the project

Every year Switzerland submits a national greenhouse gas (GHG) inventory report to the United Nations Framework Convention on Climate Change (UNFCCC), based on the Enhanced Transparency Framework, which is a central component of the Paris Agreement. The method currently used to estimate nitrous oxide (N_2O) emissions from agricultural soils under cropland and permanent grassland is relatively simple, with significant use of default emission factors (EFs) with no accounting for temporal and spatial variability of N_2O emissions. Furthermore, it does not allow estimating mitigation potentials of specific measures. The aims of this project were (i) the calibration and evaluation of the process-based model DayCent to estimate N_2O emissions from agricultural soils in Switzerland, and (ii) a first upscaling of model-based estimates of N_2O emissions to the country scale. These are significant steps towards implementing a more detailed methodology for national greenhouse gas (GHG) reporting.

2 Introduction

In about fifteen decades (1864-2016), the mean annual temperatures in Switzerland increased by 2°C, which is significantly more than the global increase of 0.9°C (FOEN, 2018). A critical consequence of this warming is a projected reduction to only 5%-37% of the 2017 glacier volume in the Swiss Alps by the end of this century (FOEN, 2022). Another harmful impact of warming is a change in the precipitation regime with higher occurrence of extreme events (*e.g.*, floods) and less snow cover (Naegeli et al., 2019). Generally, these warming-induced changes in climate variables result in a loss of biodiversity (Brito-Morales et al., 2020), disturbance of forests and agricultural land with more frequent occurrence of droughts and megadroughts (Vicente-Serrano et al., 2020; Williams et al., 2020). The increasing level of GHG emissions to the atmosphere since the pre-industrial era is the main driver of this warming (Hoegh-Guldberg et al., 2018).

The last Swiss GHG inventory showed that, in 2021, 43'374 kt CO_2 equivalents were emitted (FOEN, 2023). From this total, CO_2, CH_4 and N_2O contributed with 33'963, 5'118 and 2'894 kt CO_2 equivalents, respectively (FOEN, 2023). Agriculture is the second most important sector contributing with 13 % to the total emissions (FOEN, 2023). Considering the different GHGs, the agricultural sector is the dominant source of methane (CH_4) and N_2O emissions (83% and 55%, respectively), with only a minor contribution to carbon dioxide (CO_2) emissions (0.1%) (FOEN, 2023).

Agricultural soils are the largest source of N_2O (Fagodiya et al., 2017; IPCC, 2019). However, estimates of N_2O emissions from soils are highly uncertain. This is due to the dynamic nature of the most important soil processes producing this gas, namely nitrification and denitrification. By affecting these processes, the diversity of soils and management practices in combination with temporal and spatial variability of weather patterns lead to high uncertainty in the estimates of N_2O emissions based on generic emissions factors. This is an important issue not only for national reporting of N_2O emissions, but also for assessing the potential impacts of mitigation policies, which depend on reliable GHG budgeting. Because of the high global warming potential (GWP) of N_2O, being 273 times[1] higher than that of CO_2 in a 100-year time horizon according to the Sixth Assessment Report of IPCC (GWP100-AR6), this gas strongly impacts the total GHG budget in agricultural systems.

The methods employed in the inventories for GHG accounting vary according to the country and depend on the availability of data on soil, climate, crop production, fertilization and management. *Tier 3* is the highest level of methodological complexity and can be based on high frequency measurements or modelling. Because of the complexity and the need of detailed databases covering the whole territory of a country, including reliable weather, farming and soil data, only few countries have been able to use modeling for their GHG inventories of the agricultural sector. For N_2O emissions from agricultural soils, so far only the U.S. and Australia report the emissions based on modeling (UNFCCC, 2021).

A central reason for using ecosystem models for N_2O emission estimates in a country arises from the high cost of extensive field measurements of this gas over time (*e.g.*, for different years or decades) and over geographic regions

[1] Some estimates for inventory purposes still use GWP values based on the prior Assessment Reports of IPCC (*e.g.*, 265 based on GWP100-AR5).

(*e.g.*, drainage basins, ecoregions). Besides of this, model-based approaches can be used to assess the potential interactive impacts of different mitigation measures, such as the optimization of timing and rates of N fertilization or reduced tillage. Therefore, modeling is a potential tool for national inventories and for predicting the impact of management practices on N_2O emissions and its contribution to the GHG balance over several decades (Lugato et al., 2018). In the project LACHSIM we first tested how well N_2O emissions from agricultural soils can be represented by the process-based model DayCent and them performed a first upscaling of the model simulations of N_2O emissions to a country scale. The scope of the project is depicted in the *Figure 1* below.

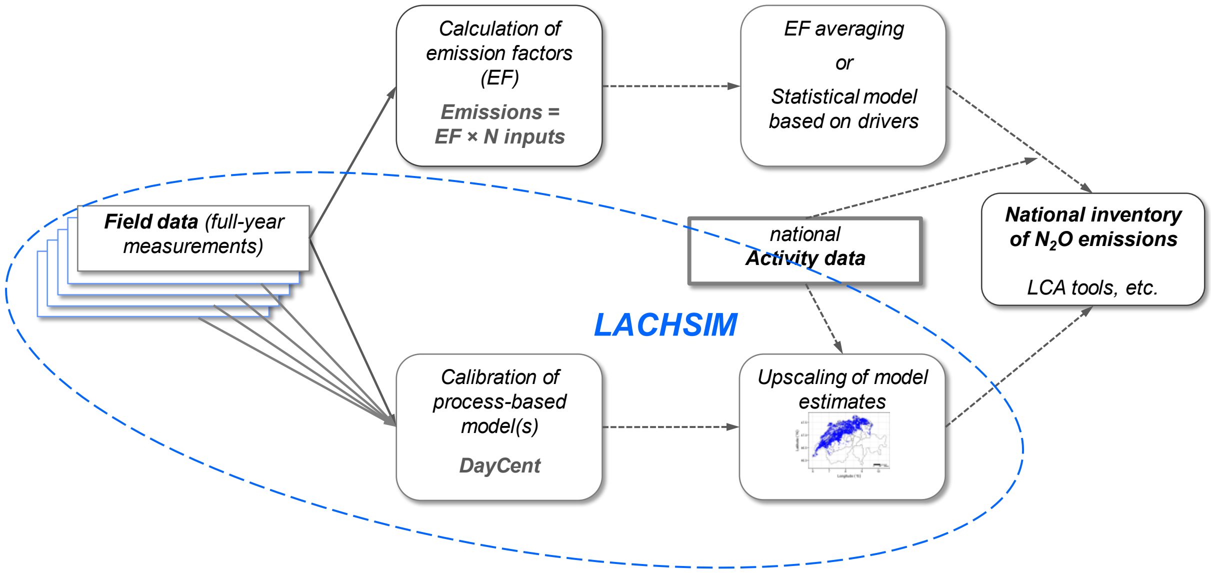

Figure 1: Representation of the LACHSIM project (outlined with blue dashed line) as a step for development of a country-specific N_2O emission inventory based on the process-based model DayCent.

3 Model selection

Many different ecosystem models have been used to predict soil N_2O emissions (*Table 1*). These models are typically based on submodels that simulate ecosystem processes including plant growth, decomposition, respiration, water fluxes, and greenhouse fluxes (Parton et al., 1998). Soil temperature and water dynamics are usually the major processes determining key ecosystem processes in the models (Grant, 1997; Izaurralde et al., 2006; Li et al., 1992). In Switzerland several models were applied to simulate N_2O from agricultural soils, mainly on permanent grassland, including ecosys (Grant et al., 2016), PaSim (Calanca et al., 2007), APSIM (Fuchs et al., 2020) and DayCent (Lee et al., 2020a; Martins et al., 2024; Martins et al., 2022; Necpalova et al., 2018).

Table 1: Process-based models commonly used for simulation of GHG emissions from natural and agricultural systems.

Abbreviation	***Model***	***Institution***	***Reference***
DNDC	The denitrification-decomposition model	University of N. Hampshire	Li et al. (1992)
ecosys	Comprehensive model of natural and managed ecosystems	University of Alberta	Grant (1997)
DayCent	Daily version of the CENTURY ecosystem model	Colorado State University	Parton et al. (1998)
PaSim	Pasture Simulation Model	Institute of Terrestrial Ecology, Edinburgh	Thornley (1998)
EPIC	Environment policy integrated climate model	University of Maryland	Izaurralde et al. (2006)
APSIM	Agricultural Production Systems Simulator	CSIRO Agriculture Flagship, Australia	Holzworth et al. (2014)

The selection of the most appropriate model depends on (i) its ability of satisfactorily represent the most important management practices and cropping systems, (ii) the large-scale availability of driving variables (model inputs) for regional scale, (iii) the possibility of calibration/validation of model output with observed data (IPCC, 2019). The complexity is also an important aspect for the selection of a model. The greater the complexity of the model, the greater is its ability to represent the simulated process (Del Grosso et al., 2019). On the other hand, higher complexity means more inputs required for the simulations. Therefore, the selection of a model for national GHG inventories depends also on the availability of required inputs to run the model for different regions. Considering the potential availability of key input data in Switzerland for N_2O simulation at the country-scale, models with an intermediate level of complexity, including DayCent and DNDC, are considered the most suitable for regional simulations.

Among models with intermediate complexity, DayCent has been successfully applied for a *Tier 3* approach in the national inventory of the U.S. (IPCC, 2019; US-EPA, 2023). It has been used for reporting N_2O emissions from mineral soils, soil organic carbon (SOC) stock changes and CH_4 emissions from rice cultivation in flooded soils (US-EPA, 2023). It has also been used to simulate the impact of different management practices or climate change scenarios on GHG emissions in different regions of the world, including Europe (Álvaro-Fuentes et al., 2017; Cheng et al., 2014; Lugato et al., 2018; Weiler et al., 2017). It stems from the CENTURY model that was broadly used to simulate SOC dynamics (Parton et al., 1987; Parton et al., 1998). For Switzerland, DayCent was successfully applied for simulations of N_2O emissions of a long-term experiment in a project conducted by the Sustainable Agroecosystem Group of the Federal Institute of Technology (ETH) in Zurich (Necpalova et al., 2018). They showed that DayCent was able to capture temporal dynamics and the scale of N_2O emissions of four different fertilization treatments rather well. Only during a phase of cover cropping, there was a mismatch between the simulated and measured N_2O emissions, which was ascribed to a lack of input data (yield or biomass of cover crops) for modelling. Another two studies conducted later by the same research group at ETH, but at a national level also applied DayCent (Lee et al., 2020a; Lee et al., 2020b). Since the suitability of a model has to be thoroughly proven and documented for national greenhouse gas reporting we decided to directly start testing DayCent. An advantage of DayCent is that the community using it is active and the model is regularly improved by researchers at Colorado State University (Hartmann et al., 2019). Therefore, an evaluation of the remaining models in *Table 1* was not conducted.

An additional important reason to use DayCent was a collaboration established with Dr. Magdalena Necpalova and Prof. Johan Six from ETH with experience with DayCent (Lee et al., 2020a; Lee et al., 2020b; Necpalova et al., 2015; Necpalova et al., 2018). They shared with us part of the parametrization previously performed for the model. For the present project, we have updated this calibration to be compatible with the latest version of DayCent (version DD17centEVI). A calibration for new crops and also for grassland categories not included in the study of Necpalova et al. (2018) was performed. Additionally, calibration was expanded to include parameters controlling N_2O losses. Several datasets of measured soil N_2O emissions under field conditions in Western Europe were included for calibration of the model and further evaluation of its predictive ability. Further details were also presented in studies developed within the scope of this project for croplands (Martins et al., 2022) and grasslands (Martins et al., 2024).

4 DayCent model

4.1 Model description

Daily Century, abbreviated as DayCent, is a biogeochemical process-based model used to simulate dynamics of vegetation growth, soil organic pools, nutrient cycling (N, P and S), CH_4 and N trace gases (Hartmann et al., 2019; Parton et al., 1998). The model accounts for the effect of management practices, including fertilization, burning, irrigation, drainage, grazing, soil cultivation and harvest (*Figure* 2). The main inputs for DayCent are (i) daily weather data, with the number of variables depending on the simulation mode; (ii) soil properties, including bulk density (BD), field capacity, permanent wilting point, minimum possible water content, distribution of roots in different layers, contents of clay, sand and SOC[2], saturated hydraulic conductivity (K_{sat}), and pH; (iii) vegetation type[3], including croplands (different annual and perennial crops), grasslands (*e.g.*, rangelands, meadows, pastures, leys), and forests (perennial and deciduous); (iv) management (type and timing), including fertilization, irrigation, drainage, tillage, sowing, harvest, and deforestation. Soil moisture and hydraulic properties that were not available for the field studies were estimated using pedotransfer functions (PTFs) based on texture, BD and SOC content (AG Boden, 2005; Saxton and Rawls, 2006).

The drivers of vegetation growth in the model are water and nutrient availability, solar radiation, air and soil temperature, and CO_2 concentration in the air. The adjustable parameters of vegetation growth in the model are related to photosynthetic radiation-use efficiency, plant phenological patterns, and shading by dead vegetation. The effect of shading by trees is only possible in simulations with savannas, which are not present in this study. The simulation of total SOC stocks in the model is controlled by the dynamics of three conceptual soil organic pools (Parton et al., 1987). The first organic pool is an active pool, which is composed of microbial biomass and other very labile organic compounds and presents and turnover rate of months to a few years. The second is a slow organic pool with moderate resistance to decomposer activity due to physical and biochemical protection and has a turnover rate of a couple of years to a few decades. The third is a passive organic pool, which is the fraction that is considered stable in the soil, with residence times usually longer than 1000 years (Martel and Paul, 1974). The dynamics of carbon and other nutrients (N, P and S) in these pools depend on the input rates and amounts of these elements in each pool, as well as decomposition rates influenced by soil temperature, water content, and texture (Del Grosso et al., 2011; Hartmann et al., 2019; Parton et al., 1987). The N availability for plant uptake, nitrification, and denitrification, is estimated as a function of external N inputs (mineral or organic fertilization and atmospheric N deposition), N mineralization from soil organic N stocks and plant residues, and biological N_2 fixation (BNF). The model assumes that biological N_2 fixation (i) only occurs when the level of mineral N is not sufficient for plant growth and (ii) has its rates limited to a maximum value, which can be adjusted according to the vegetation type[4].

In the model, nitrification and denitrification are the processes resulting in the fluxes of N_2O, nitric oxide (NO), and dinitrogen (N_2). Field capacity, BD, minimum possible water content, and pH are soil properties used for the simulation of nitrification. Daily fluxes of N gases produced by nitrification over time are simulated as a function of water content, temperature, and ammonium (NH_4^+) content in the top 15-cm soil layer (Del Grosso et al., 2019; Hartmann et al., 2019). Texture, BD, and field capacity are soil properties used for simulation of denitrification. Daily fluxes of N gases produced by denitrification are simulated using soil nitrate (NO_3^-) availability (*i.e.*, electron acceptor), simulated heterotrophic respiration as an indicator of labile C availability (*i.e.*, electron donor), and water-filled pore space (WFPS) in each soil layer. The latter is used as indicator of soil aeration status, *i.e.*, the higher the value of WFPS, the lower is the level of O_2, which is then replaced by NO_3^- in the role of dominant electron acceptor for denitrification. In DayCent denitrification occurs, by default, at WFPS above 60%. The amount of N_2O emissions derived from denitrification is calculated from the sum of N_2 and N_2O produced and from the N_2:N_2O ratio, which ranges from 1 to 23 and depends on the ratio of NO_3^-:labile C and soil gas diffusivity.

[2] SOC content is only required as input for the simulation of soil temperature dynamics, *i.e.*, not for the simulation of soil organic pools and SOC stocks.

[3] The last versions of DayCent also allows the simulations of mixtures of both a crop/grass type and a tree/shrub type (savanna system).

[4] Further details on the parameter controlling BNF will be presented later in Section *9.1*.

Nitrogen leaching is simulated in the model including both mineral N (only NO_3^-) and organic N forms. Leached organic N comes from the active soil organic pool mentioned above. It is assumed that the soil sand content controls the leaching intensity of both mineral and organic forms. Nitrogen leaching from a given layer is assumed to occur only when there is available N in the respective layer and when there is water flow from this layer to a lower layer.

We performed the DayCent simulations using the "weather extra drivers" mode, which is based on the use of daily values of precipitation, maximum and minimum air temperature, solar radiation, air relative humidity and wind speed. We used weather data recorded at each site, which we gap-filled based on meteorological stations located nearby. For example, in Switzerland, data from nearby stations were available on the Data Portal for Teaching and Research (IDAweb) portal of the Swiss Federal Office of Meteorology and Climatology (MeteoSwiss) (https://gate.meteoswiss.ch/idaweb).

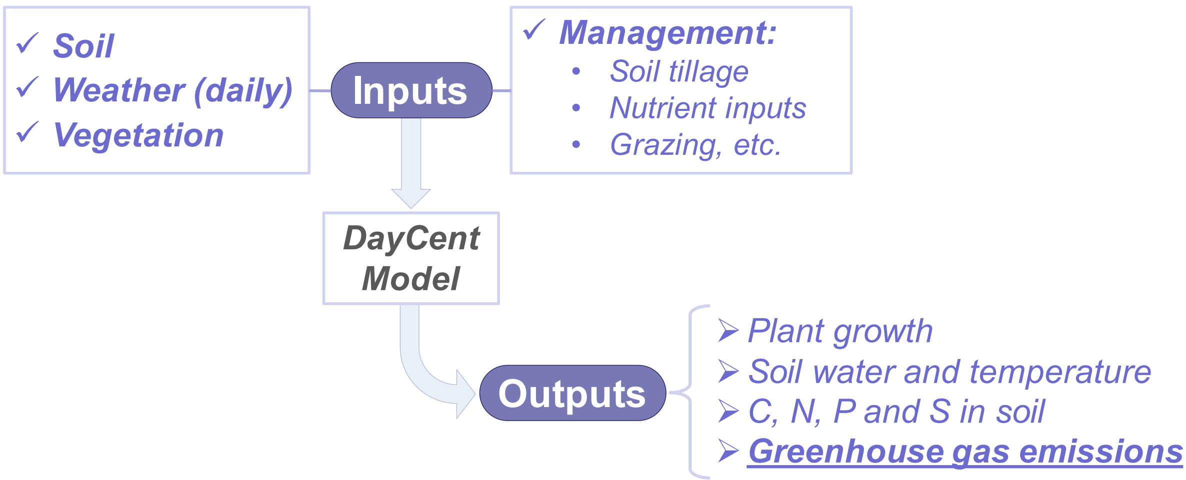

Figure 2: Basic representation of workflow of DayCent simulations; detailed description of the model is provided by Hartmann et al. (2019).

4.2 Model initialization

The initialization of the model, also referred to as spin-up, consisted of a simulation of the C and N cycling over many centuries to define the size of different soil organic pools before starting simulations for the recent experimental period. For this model initialization, a pattern of land-use history at the locations of the experimental sites used in the present project in Switzerland, France and Germany, during the last two millennia was based on information from the literature with a focus on Western Europe (ANL, 2014; Bürgi, 2016; Kapfer, 2010; Vannière et al., 2003). The overall assumptions were consistent with those previously used by Necpalova et al. (2018). We considered usually 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 (Necpalova 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, frequency of harvest on grasslands, were considered over these phases. The meteorological data from each field study were used with recursion for the initialization of the model, *i.e.*, data were repeated in a loop for centuries prior the modern phase.

5 Long-term experiments used for model calibration

The use of model-based GHG emission estimates requires an acceptable uncertainty that is conditioned upon a thorough calibration of the model followed by evaluation (IPCC, 2019). The process of calibration of a model is an adjustment of the mathematical parameters to produce a final output within an acceptable deviation from the real observed values. To adopt a *Tier 3* approach, the model parametrization must be country-specific rather than using default parameters (IPCC, 2019). It is expected that the better the calibration is, the better is the power of the model prediction for a given region, *i.e.*, the closer are the modeled data to the real observations. An evaluation of the model performance for independent sites is also a necessary step towards using modeling for N_2O emission estimates in a country. Therefore, the calibration and evaluation of a model depends on the availability of reliable field data for comparison with the model output. It is important also to consider that the complexity of agricultural systems used in Switzerland, with diverse types of nutrient inputs, with grasslands under multiple categories of use and croplands based on diverse crop rotations and soil management makes the use of process-based models for the estimation of N_2O emissions challenging. Therefore, the use of field data to calibrate and evaluate the model for Swiss conditions is especially important.

In our project, the Swiss datasets from field experiments were expanded to Western Europe, presenting similar soil and weather conditions to those in Switzerland, to assess the performance of DayCent for prediction of N_2O emission from agricultural soils under typical management practices used in this country. We focused on croplands during the first phase of the project and on permanent grasslands in the second phase. As a first step to test DayCent for each one of these two land-use categories we searched the literature for studies with measurements of soil N_2O fluxes from field experiments. The purpose was to find field studies where:

- the measurements of N_2O emissions were performed under pedoclimatic conditions and agricultural management representative for or similar to those of Switzerland;
- a reliable strategy of N_2O monitoring was adopted – the studies using chambers had to meet a set of criteria defined by Rochette and Eriksen-Hamel (2008) for quality control of N_2O flux measurements (*e.g.*, minimum chamber height, insertion in soil, sampling time);
- data of an auxiliary variable related to soil water content (usually WFPS) were available, considering the importance of this variable for processes of N transformation in soil (nitrification and denitrification).

Based on this survey, we started to contact researchers in Switzerland and nearby countries to ask whether they would be willing to share their data. Datasets from sites in Switzerland, France and Germany were shared with us for the LACHSIM project. The location of the field studies used in the present project are located in the *Figure 3*.

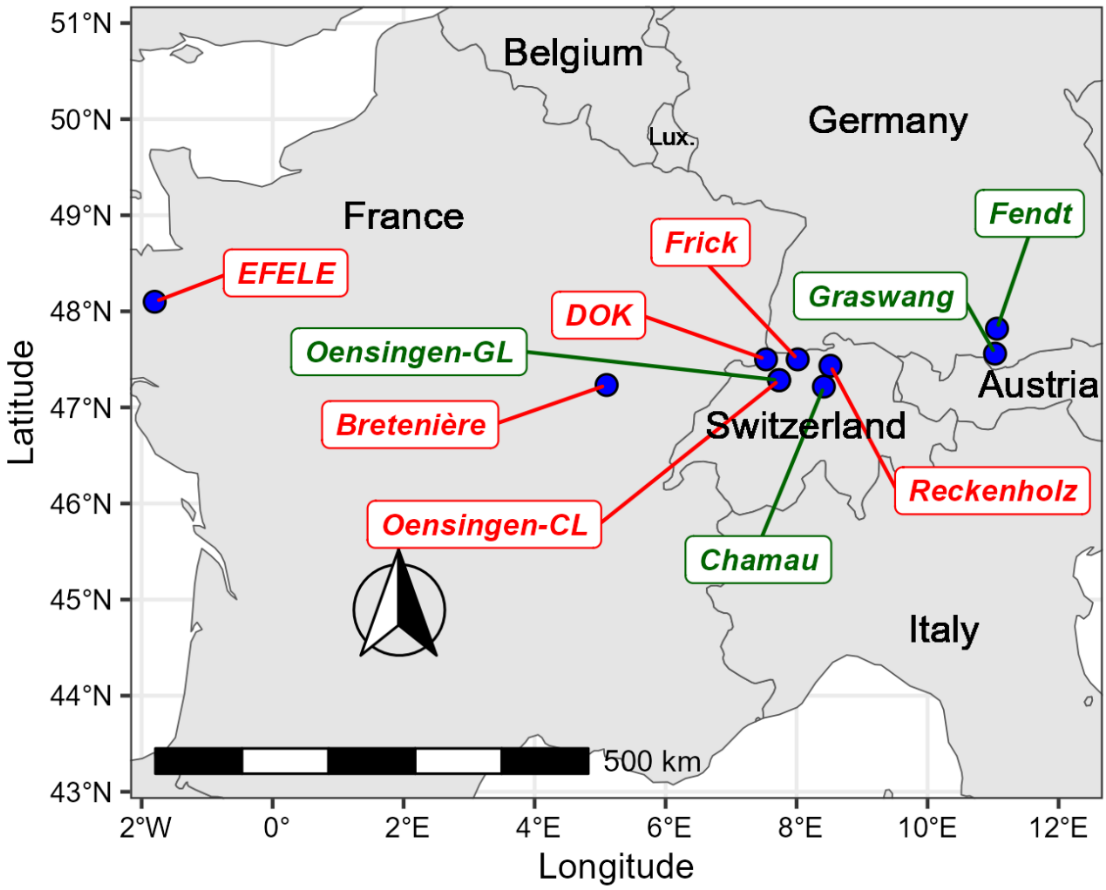

Figure 3: Location of the field studies used for calibration and validation of the DayCent model for cropland (red) and grassland (green) sites.

5.1 Cropland sites

The measurement data of six sites were used for the calibration and evaluation of the DayCent model (sites marked in red in *Figure 3*). The most important soil and weather characteristics of the sites are presented in *Table 2*. Soil properties available at the plot level were used as input data for each modeled treatment. Approximately 24,000 daily N_2O flux observations in cropland sites were included in this phase of the project LACHSIM considering the frequency of sample collection and the number of chambers per treatment in each field study. Some details of the N_2O flux measurements in the different field studies are presented in *Table 3*. The crops used in the field studies are among the most important in terms of harvested area in Switzerland (FAOSTAT, 2022). The N fertilization rates per crop cycle during the N_2O flux monitoring across different field studies and treatments ranged from 0 to 335 kg N ha^{-1}. Details describing the crop rotations at each field study are presented in *Table 3*.

5.1.1 Experimental sites in Switzerland

The long-term field study known as DOK is located in Therwil, Switzerland. DOK is the German acronym for *"Dynamisch, Organisch, Konventionell*" which stands for dynamic, organic and conventional. This study is set up 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 N_2O simulations with DayCent 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, and the use of agents approved for organic farming (*e.g.*, copper and bacillus thuringiensis), while in the non-organic systems herbicides, fungicides and pesticides are applied (Knapp et al., 2023).

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 N_2O monitoring. The organic fertilization treatments were (i) cattle slurry alone (referred to as Slurry) and cattle manure compost plus slurry (Manure compost). The soil tillage treatments were (i) conventional tillage (15–18 cm, 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) (Emmel et al., 2018), the ecosystem-scale N_2O fluxes were measured in 2019 at high temporal resolution (10 Hz) using the eddy-covariance technique (Maier et al., 2022). For the present study, the N_2O 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 at Reckenholz in Zurich was conducted for one cropping season in 2014 to test the effect of biochar and limestone application on N_2O emissions from a soil under maize (Hüppi et al., 2015). The treatments consisted of different 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 three times after sowing at rates ranging from 40 to 80 kg N ha^{-1}.

5.1.2 Experimental sites in France

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., 2016; Vermue et al., 2016). It involves different crop rotations, intensities of tillage and herbicide applications. Originally, five different treatments were applied in different plots, without replication (Chikowo et al., 2009). Measurements of N_2O 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 without herbicides, *i.e.,* with weed control based solely on physical and cultural practices, including in-crop mechanical weeding, use of crops more competitive against weeds and soil tillage only when necessary. Soil N_2O 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 N_2O 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 N_2O emissions were performed using 3 chambers per treatment.

Table 2: Climate and soil[1] characteristics of the six cropland sites used for simulations with DayCent.

Field study	Location	Coordinates	Altitude (m a.s.l.)	MAP (mm)	MAT (°C)	Soil Class (FAO-WRB, 2015)	Clay (%)	Silt (%)	Sand (%)	pH	SOC (%)	BD (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

[1] Average of plots used for the simulations (plough layer). MAP: mean annual precipitation; MAT: mean annual temperature; SOC: soil organic carbon; BD: bulk density.

Table 3: Crop rotations and details regarding N_2O measurements of the six field studies used for simulations with DayCent.

Field studies	Period of the study [1]	Crop rotation in the last ten years used for simulations [2]	Period of N_2O flux measurements	Method of N_2O flux measurements	References [3]
Bretenière	2000-2013	*Treatment S1ᵈ:* WB_{04}–RP_{05}–WW_{06}–WB_{07}–RP_{08}–WW_{09}–WB_{10}–RP_{11}–**WW_{12}–WB_{13}**; *Treatment S2:* RP_{04}–WW_{05}–OA_{05}–SB_{06}–SY_{07}–WW_{08}–RP_{09}–SY_{10}–WW_{11}–**SB_{12}–OA_{12}**–SY_{13}; *Treatment S3:* MU_{03}–WW_{04}–RP_{05}–TR_{06}–SY_{07}–WW_{08}–RP_{09}–TR_{10}–RP_{11}–**WW_{12}–CC_{12}**–SY_{13}; *Treatment S5:* WB_{04}–FB_{05}–TR_{06}–RP_{07}–WW_{08}–WB_{09}–CC_{09}–FB_{10}–WW_{11}–**AF_{12}**–MZ_{13}	Mar. 2012–Apr. 2013	Chambers with automated sampling	Chikowo et al. (2009); Ugarte Nano et al., 2015, 2016; **Vermue et al. (2016)**
EFELE [4]	2012-2020	*All treatments:* **WW_{13}–CC_{14}–MZ_{14}–WW_{15}–CC_{16}–MZ_{16}–WW_{17}–CC_{18}–MZ_{18}– WW_{19}–CC_{20}–MZ_{20}**	Mar. 2013–Sep. 2020	Chambers with automated sampling	INRAE (2021)
DOK	1977-2014	*All treatments:* GC_{05}–MZ_{06}–WW_{07}–GM_{08}–SY_{08}–RY_{09}–PO_{09}– WW_{10}–GC_{11}–**GC_{12}–MZ_{13}–GM_{14}**	Aug. 2012–Mar. 2014	Chambers with manual sampling	Mäder et al. (2002); Mayer et al. (2015); **Skinner et al. (2019)**
Frick	2002-2014	*All treatments:* SP_{05}–GC_{06}–GC_{07}–MZ_{08}–WW_{09}–CC_{10}–SF_{10}– SP_{11}–**GC_{12}–GC_{13}–WW_{14}–CC_{15}**	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}–**WW_{19}–WB_{20}**	Jan. 2019–Jan. 2020	High resolution eddy covariance system	Emmel et al. (2018); Revill et al. (2019); **Maier et al. (2022)**
Reckenholz [4]	2014	*All treatments:* **MZ_{14}**	Mar. 2014–Dec. 2014	Chambers with automated sampling	**Hüppi et al. (2015)**

[1] Period from the beginning of the experiment to the last year of simulation, *i.e.*, not necessarily to the end of the experiment.
[2] Letters indicate the crop type 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: silage or grain 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 N_2O fluxes were measured.
[3] The studies cited in bold present more details of the N_2O measurements and results comparing the treatment effects.
[4] Please note that the simulations for EFELE and Reckenholz field studies were performed for less than 10 years due to the shorter duration of these experiments.

5.2 Grassland sites

Field data from long-term experiments in four permanent, temperate grassland sites located in Switzerland and Germany were used in the present project. Two sites are located in the Swiss Plateau and the other two in the pre-alpine region of Bavaria, Southern Germany (sites marked in green in *Figure 3*). At each site, the grasslands were subjected to different management practices regarding the intensity of cutting and N fertilization inputs, as described further below. Description of soil, weather, management treatments and measurements are presented in the *Table 4* and *Table 5*.

5.2.1 Experimental sites in Switzerland

The first grassland site is located in Chamau (393 m a.s.l.), in the canton of Zug, in the valley of the Reuss River. Two adjacent plots have been used in this experiment since 2002 (Fuchs et al., 2018; Merbold et al., 2021; Zeeman et al., 2010). One of the plots was used as a control, with mowing events from four to six times per year, sporadic grazing, and slurry application as the most usual fertilization practice. The other plot, hereafter referred to as clover treatment, was subjected to a greenhouse gas mitigation management after 2014. It consisted of over-sowing the plot with clover in each spring associated with zero N-fertilizer application. The purpose of this management was to increase the proportion of clover to grass and therefore provide more N to vegetation via BNF. In contrast, slurry was applied at N rates of 311 kg ha^{-1} in 2015 and 181 kg ha^{-1} in 2016 on the control plot. The eddy covariance flux tower used for N_2O measurements was located on the border between the two adjacent areas with more than 2 ha each. The system was equipped with a quantum-cascade laser absorption spectrometer (QCLAS) to measure the concentration of N_2O and a sonic anemometer to measure wind speed and direction (Fuchs et al., 2018; Merbold et al., 2014). High temporal resolution data (10 values per second) were converted to daily N_2O fluxes to match the temporal resolution of DayCent outputs.

The second grassland site is located in Oensingen (450 m a.s.l.), in the canton of Solothurn. The experimental area was converted from an arable field to permanent grassland in 2001 and was subdivided into two adjacent plots of 0.76 ha each. The first plot was then subjected to an intensive management and the second plot to an extensive management (Ammann et al., 2007, 2009, 2020). The plot under intensive management was fertilized with slurry or mineral N fertilizer, mostly ammonium nitrate. The average annual N fertilization rates were around 200 kg ha^{-1}. The N fertilizer was applied some days after harvest or at the beginning of vegetation growth in each year. The plot under extensive management received no fertilizer during the entire experimental period. Another aspect differentiating the management of the two plots was the mowing regime, with more cuts per year under the intensive management (4-5 *vs.* 2-3 times per year respectively). The measurements of N_2O on the grassland plots were performed using eight automatically operated chambers per plot (Ammann et al., 2009; Flechard et al., 2005). The N_2O concentration in the headspace of the chambers was analyzed using either a photoacoustic technique or a gas filter correlation technique. Nitrous oxide emissions were monitored from 2004 to 2010. In the present study, only the years before a renovation in 2008 were included in the simulation.

Table 4: Climate and soil[1] characteristics of the four grassland sites used for simulations with DayCent.

Field study location	Coordinates	Altitude (m a.s.l.)	MAP [2] (mm)	MAT [3] (°C)	Soil Class (FAO-WRB, 2014)	Clay (%)	Silt (%)	Sand (%)	pH	SOC [4] (%)	BD [5] (g cm^{-3})
Chamau, Switzerland	47°13'N, 8°25'E	393	1151	9.1	Gleysol-Cambisol	19	45	36	6.5	2.8	1.1
Oensingen, Switzerland	47°17'N, 7°44'E	452	1086	9.8	Eutri-stagnic Cambisol	43	47	10	6.4	2.1	1.23
Fendt, Germany	47°49'N, 11°4'E	600	1033	8.6	Cambic Stagnosol	31	42	27	5.8	2.2	1.3
Graswang, Germany	47°34'N, 11°2'E	860	1398	6.5	Fluvic Calcaric Cambisol	51	39	9	6.7	3	1.07

[1] Average of plots used for the simulations (plough layer). MAP: mean annual precipitation; MAT: mean annual temperature; SOC: soil organic carbon. BD: bulk density.
[2] Soil properties represent the 0-30 cm layer (values used as model inputs).

Table 5: Description of the N_2O measurements of the six field studies used for simulations with DayCent.

Field study location	Period of simulation [1]	Management treatments	Period of N_2O flux and/or N leaching measurements [2]	References
Chamau, Switzerland	2001–2016	Control *vs.* mitigation based on oversowing with clover	Jan. 2013–Dec. 2016	Fuchs et al. (2018), Merbold et al. (2021)
Oensingen, Switzerland	2001–2007	Intensive *vs.* extensive	Mar. 2004–Dec. 2007	Ammann et al., (2007, 2009, 2020)
Fendt, Germany	2011–2021	Intensive *vs.* extensive	Jan. 2012–Dec. 2014	Fu et al. (2017), Lu (2016), Kiese et al. (2018)
Graswang, Germany	2011–2021	Intensive *vs.* extensive	Jan. 2012–Dec. 2014	Fu et al. (2017), Lu (2016), Kiese et al. (2018)

[1] Years with renovation of grasslands were not included in the model calibration and evaluation, considering that it is not typical management practice in Western European grasslands.
[2] Period considered in the present project.

5.2.2 Experimental sites in Germany

The grassland sites in Fendt (600 m a.s.l.) and Graswang (860 m a.s.l.) are part of the Terrestrial Environmental Observations (TERENO) observatory in Southern Germany (Kiese et al., 2018). The experiments consisted of lysimeters filled with undisturbed soil cores (1.0 m^2, 140 cm depth) from each site (elevation). In the present study, we considered only six lysimeters with soil excavated and placed at the same site. The original grassland vegetation was preserved in the lysimeters (Fu et al., 2017). During the experiments, three of the lysimeters at each site were submitted to an intensive management and the other three to an extensive one. Therefore, the experiment was conducted with three replicates. The management differed in regard to the number of mowing and fertilization events per year. The lysimeters under extensive management were submitted usually to three mowing events and received one or two slurry applications (totaling up to 42-84 kg N ha^{-1} per year) while lysimeters under intensive management had usually four or five mowing events and received multiple slurry applications totaling up to 210-256 kg N ha^{-1} per year (Kiese et al., 2018).

Tensiometers were used to measure the water potential at the bottom of each lysimeter and, concurrently, at three reference plots at the same depth (140 cm). Adjustments in soil water content at the bottom of the soil were performed to ensure that the water dynamic inside the lysimeter was the same of that outside. Pressured suction cups connected to 1.0-L glass bottles were used to collect soil solution. The total amount of N leaching was determined by combining the amounts of seepage water and estimates based on the concentration of N from the samples collected using the suction cups. More details are presented in Fu et al. (2017).

At Graswang, the N_2O measurements were made using manual gas sampling with polypropylene syringes during 3 years (2012 to 2014). At Fendt, manual sampling was carried out from January until May 2012 and, after that period, a robotic gas collection system was installed to automatically execute the gas sampling. The concentration of N_2O in the samples collected manually were analyzed using gas chromatography after transferring the gas samples from the syringes to glass vials. The concentration of N_2O in the headspace of the automatic chambers was analyzed online using QCLAS. The chambers had the same diameter of the lysimeter, thus covering its entire surface. The automatic chambers were 80 cm high and the manual chamber 30 cm. Manual sampling was performed with a frequency from 2 to 4 times per week. Automatic sampling was performed usually every 4 hours.

6 Model calibration

The model calibration at each site was performed by coupling DayCent with PEST (*Figure 4*). 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 the best fit, *i.e.*, minimization of difference between the modeled and observed values (Doherty, 2020). For 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.

To perform the calibration, we selected the same plant and management parameters sensitive to measured data as found by Necpalova et al. (2018). Considering the significant correlation between many parameters they found, 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 subsequent stages:

- *Stage I*: the parameter denoting the photosynthetic radiation-use efficiency in the forest phase was calibrated during model initialization based on initial SOC stocks observations in the top arable layer at a 20 cm depth at each field study.
- *Stage II:* plant 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[5];
- *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/or crop yield data.
- *Stage V:* N cycle parameters controlling nitrification and denitrification were calibrated based on observed cumulative N_2O emissions over time.

Linear interpolation was used for gap filling of daily measured N_2O 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 N_2O emissions. Likewise, the modeled daily N_2O fluxes corresponding to the unfilled gaps were also excluded from the modeled cumulative N_2O emissions used in the calibration process. By contrast, for coupling DayCent and PEST for calibration of the N cycle parameters at the stage V described above, new selected datasets were created with simulated N_2O 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 Necpalova et al. (2015, 2018).

[5] This step was only used in croplands, considering that soil cultivation (*e.g.*, seedbed preparation) is not a typical management practice in permanent grassland areas in Switzerland.

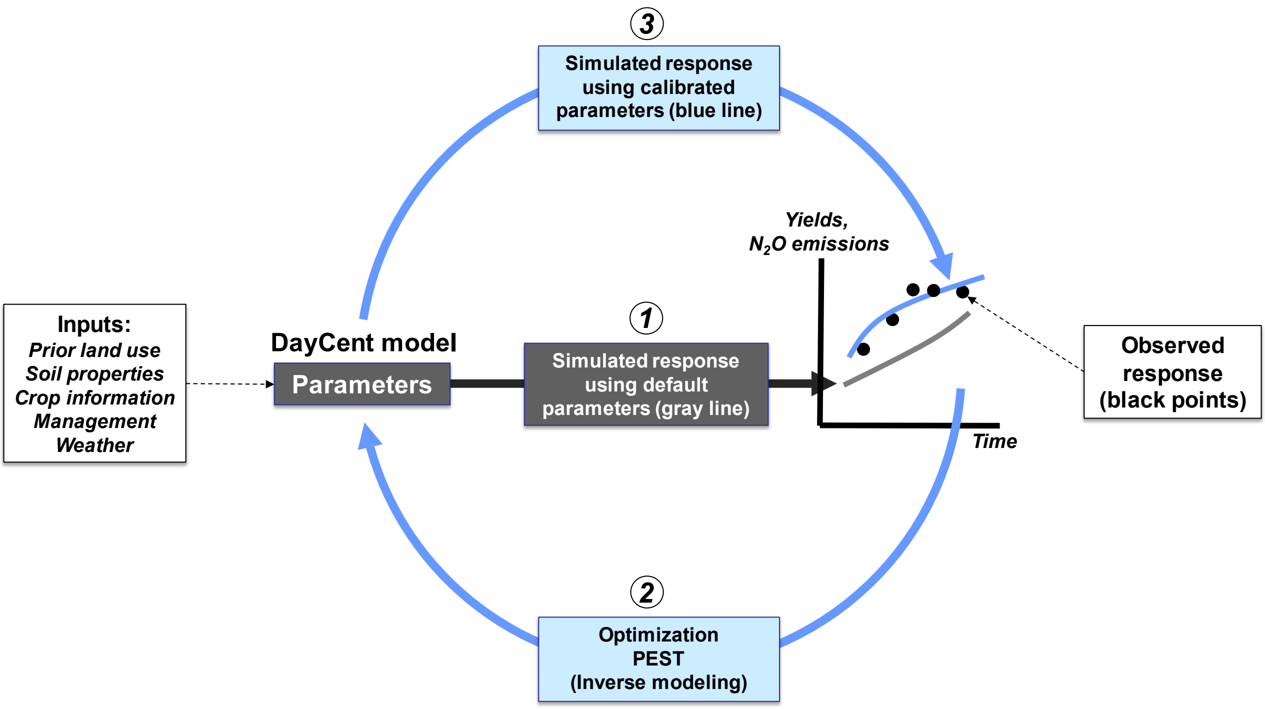

Figure 4: Procedure for calibration of DayCent parameters based on field data from cropland and grassland sites.

By selecting only crop cycles (or an entire year in case of grasslands) with entire gap-filled management periods for N_2O flux measurements, we made a comparison of DayCent estimates against estimates based on EF approaches commonly referred to as IPCC *Tier 1.* The latter represents the most basic method for national inventories of greenhouse gas emissions and hardly includes country-specific data. Further details related to the EF approach applied here can be found in the Appendix I for croplands and Appendix II for grasslands.

In addition to the observed N_2O emissions for each site, we used observed yield data to assess the overall performance of the model, *i.e.*, as a general quality control of the model outputs (Del Grosso et al., 2020). Evaluating yields in the different stages of the calibration procedure was also an attempt to reduce the risk of a good model performance for N_2O emissions despite errors in parameters not directly related to the N cycle (*e.g.,* parameters related to plant production). More insights on the equifinality, *i.e.*, good model fit obtained for the wrong reasons, was given by Beven (2006).

7 Model evaluation

7.1 Leave-one-out procedure

After calibration of the model for each site, we also performed a leave-one-out (LOO) cross-evaluation to assess the ability of DayCent to simulate soil N_2O emissions for new independent sites. The cross-evaluation is a procedure to assess the predictive ability of the model, *i.e.,* to make out-of-sample predictions. Cross-evaluations were carried out separately for each land use category, *i.e.* one for cropland and another for grasslands. For each land use category, the cross-evaluation was based on alternately splitting the datasets in one site for evaluation and the remaining sites for calibration. In this way, the simulations for each site were carried out by applying the average value of the calibrated parameters obtained for the other sites. This means that the optimized parameters for a given site were excluded from the average parameters calculated for the same site. More details of this procedure were previously described by (Wallach et al., 2014). As example, the LOO cross-evaluation procedure is illustrated for cropland sites in *Figure 5*.

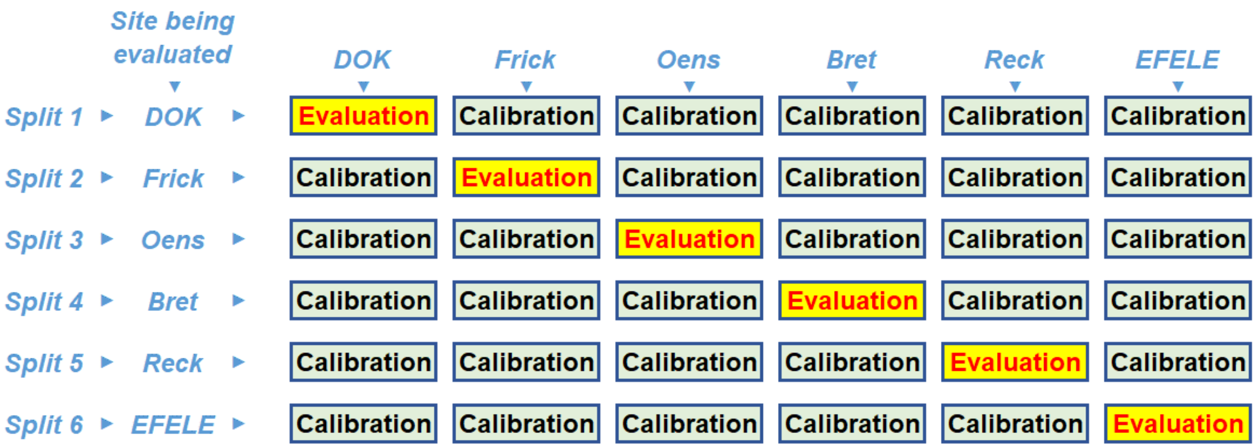

Figure 5: Scheme for leave-one-out (LOO) cross-evaluation of the performance of DayCent based on observed field data.

7.2 Statistical metrics

Linear regressions of modeled against observed values were used to assess the performance of the model. Average values were used for obtaining a single value for treatments with field replicates (see *Section* ***Fehler! Verweisquelle konnte nicht gefunden werden.*** **Fehler! Verweisquelle konnte nicht gefunden werden.**). 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* values are 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* indicate greater accuracy of 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 RStudio (Campbell, 2019) was used to develop a script to run DayCent for each site and instantaneously obtain the figures and data outputs for assessing the performance of DayCent during calibration and evaluation stages.

8 Performance of DayCent for croplands

8.1 Site-specific calibration and simulation of daily N_2O fluxes

The ability of DayCent to reproduce daily N_2O fluxes before and after site-specific calibration is presented in the *Figure 6* to *Figure 11*. Site-specific calibration effectively improved the agreement between modeled and observed daily N_2O fluxes that are affected by crop types, amount and type of N inputs and soil tillage. To illustrate this with an example, the conventional and the no-tillage treatments at Bretèniere are used (*Figure 6a-b*). At this site simulations with the uncalibrated model showed some fertilizer-induced N_2O pulses up to 34 g N ha^{-1} d^{-1} during the wheat-growing season under conventional tillage, while the observed fluxes stayed below 10 g N ha^{-1} d^{-1} (*Figure 6a*). Conversely, the uncalibrated model significantly underestimated the high N_2O fluxes in the no-tillage treatment, which were up to 246 g N ha^{-1} d^{-1} after fertilization of barley (*Figure 6b*). The site-specific calibration substantially improved the ability of DayCent to capture the effects of these contrasting managements on N_2O emissions (*Figure 6a-b*). This improvement is evident by comparing the cumulative N_2O emissions (lower panels in *Figure 6a-b*). The observations reached 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 differences between modeled and 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, differences were strongly reduced and had a value of 0.8 kg N ha^{-1} for the reference and -0.1 kg N ha^{-1} for the no-tillage treatment.

Another key example that can be considered for demonstrating the calibration-induced improvement of the model were the results for Frick. The site-specific calibration for Frick clearly improved simulations of DayCent by reducing overpredicted cumulative N_2O emissions (*Figure 8*). Although some N_2O pulses associated with slurry applications (labeled *S*) and rotary tillage (labeled *rt*) were still underpredicted after calibration, the modeled cumulative emissions were significantly better after site-specific calibration. Overall, this improvement in the adjustment for cumulative N_2O emissions was also found for the other field studies. The two exceptions to this were the fully integrated weed management treatment at the Bretenière site (*Figure 6d*) and the ammonium nitrate treatment at the EFELE site (*Figure 7*). It indicates a small trade-off, *i.e.,* the overall improvement in model performance for a field experiment resulted in a slight reduction in performance in some treatments for which the model was performing well even with no calibration. In contrast, it is also worth noting that for the treatments BIOORG, CONMIN, and CONFYM of the DOK field study, even the uncalibrated model simulated the cumulative emissions well (

*Figure **9***). On the other hand, in this field study, we observed the largest relative deviation between modelled and observed N_2O emissions in the control treatment (NOFERT), even after calibration. Despite the underestimation, the lower modelled N_2O fluxes in this treatment are consistent with no N-fertilizer inputs for several decades (Mäder et al., 2002; 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 an 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.

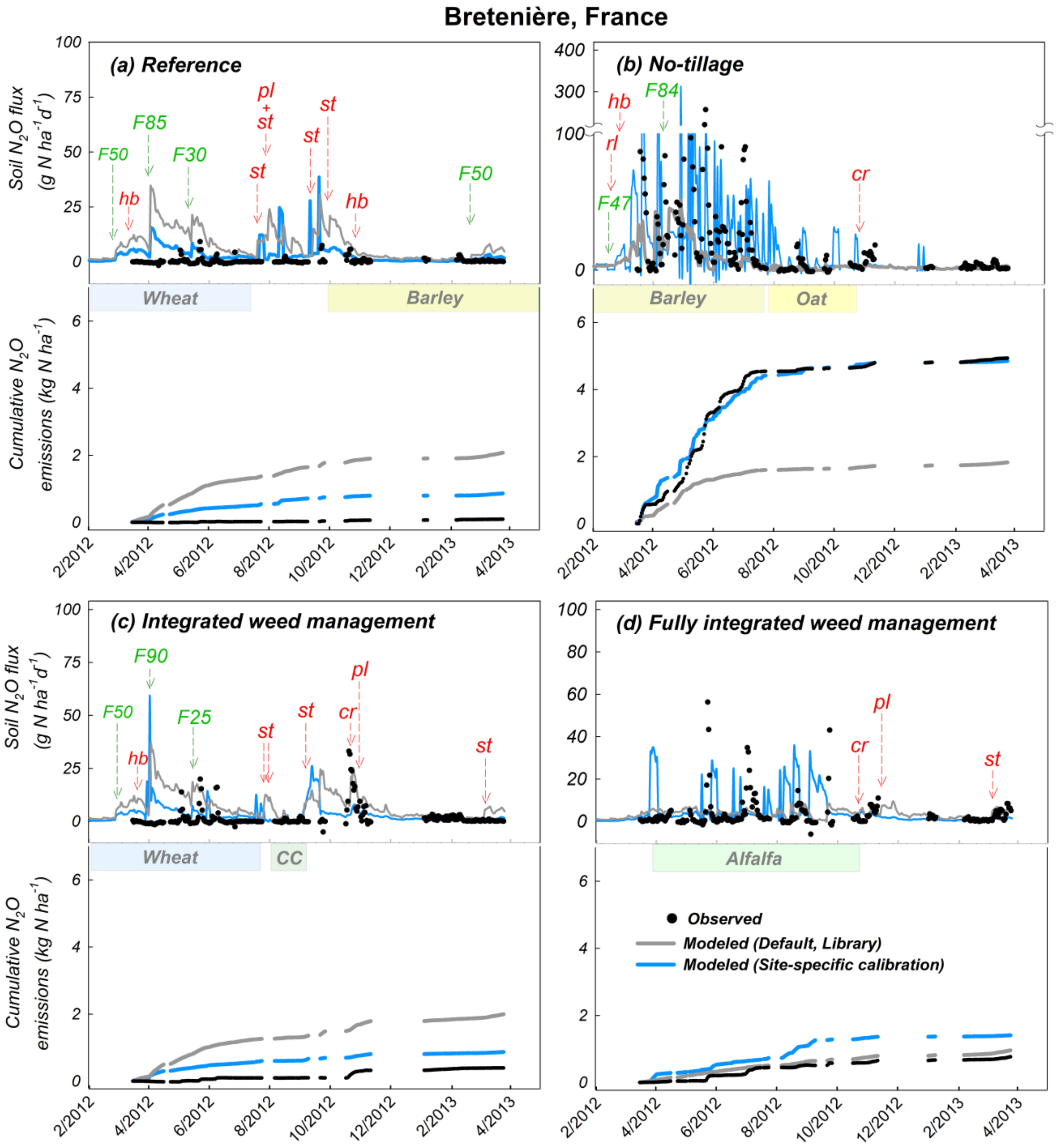

Figure 6: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the following treatments in Bretenière (France): 'Reference' (a), 'No-tillage' (b) 'Integrated weed management' (c) and 'Fully integrated weed management' (d).
Arrows associated with lowercase letters indicate cultivation events (cr: cover crushing, hb: herbicide, pl: moldboard plowing, rl: rolling, st: shallow tillage). Arrows associated with uppercase letters followed by values indicate N inputs, including fertilization type (F: synthetic fertilizer) 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}). The crop growing periods from sowing to harvest or termination are indicated below the X-axis of the upper panels; empty spaces indicate non-growing periods. CC: cover crop.

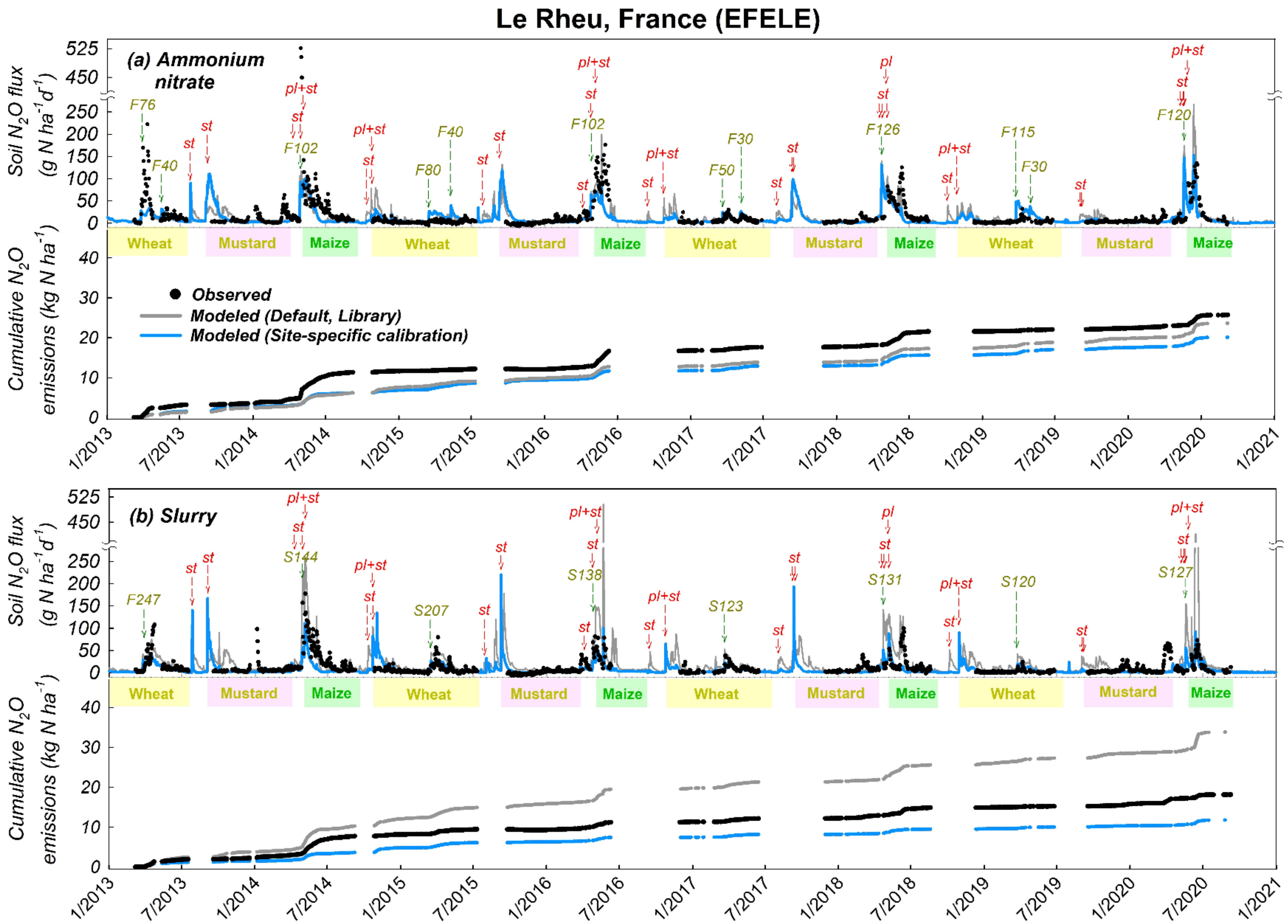

*Figure **7:** Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the following treatments of the Le Rheu (EFELE) field study (France): 'Ammonium nitrate' (a) and 'Slurry' (b). Arrows associated with lowercase letters indicate cultivation events (pl: moldboard plowing, st: shallow tillage). Arrows associated with uppercase letters followed by values indicate N inputs as synthetic fertilizer, in kg N ha^{-1} (e.g., F76 indicates an application of synthetic fertilizer at a rate of 76 kg N ha^{-1}). The crop growing periods from sowing to harvest are indicated below the X-axis of the upper panels; empty spaces indicate non-growing periods.*

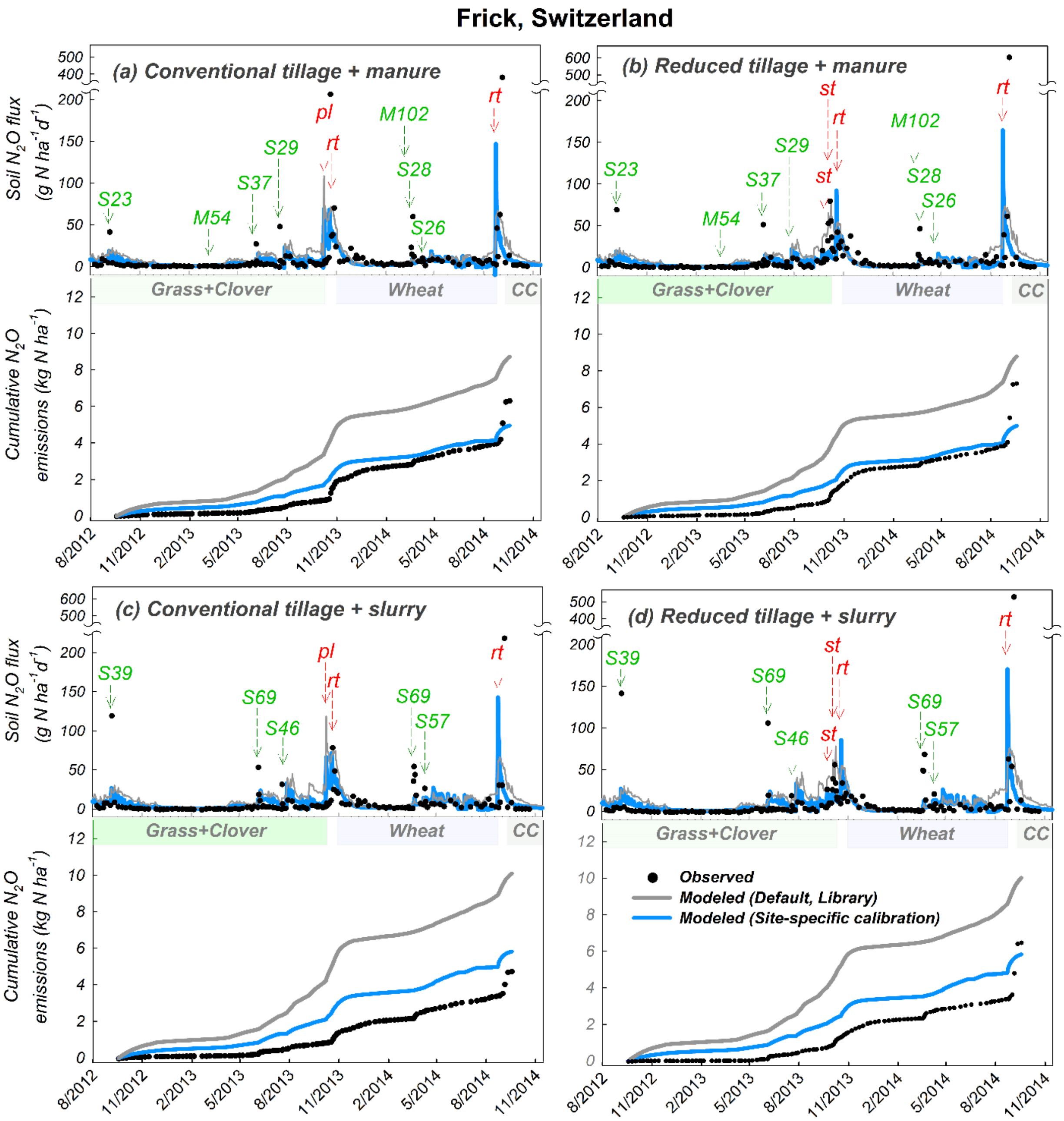

Figure 8: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the following treatments in Frick (Switzerland): 'Conventional tillage + manure' (a), 'Reduced tillage + manure' (b), Conventional tillage + slurry' (c) and 'Reduced tillage + slurry' (d).
Arrows associated with lowercase letters indicate cultivation events (cr: cover crushing, pl: moldboard plowing, rt: rotary tillage, st: shallow tillage). Arrows associated with uppercase letters followed by values indicate N inputs, including fertilization type (S: slurry or M: manure compost) and rates, in kg N ha^{-1}, respectively (e.g., S39 indicates slurry application at a rate of 39 kg N ha^{-1}). The crop growing periods from sowing to harvest or termination are indicated below the X-axis of the upper panels; empty spaces indicate non-growing periods. CC: cover crop.

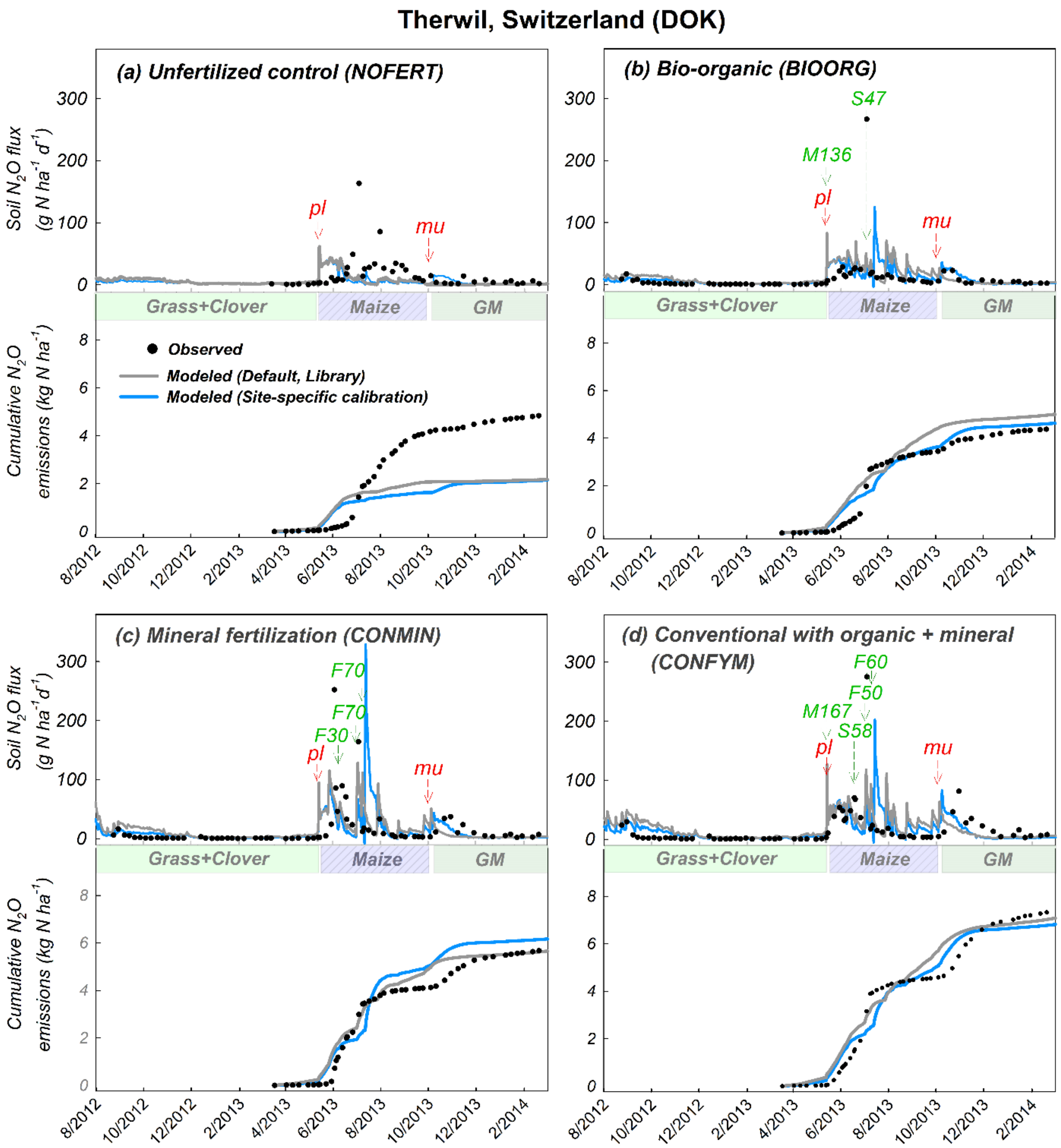

Figure 9: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the following treatments of the DOK long-term field study at Therwil (Switzerland): 'Unfertilized control' (a), 'Bio-organic' (b), 'Mineral fertilization' (c) and 'Conventional (organic + mineral)' (d).
Arrows associated with lowercase letters indicate cultivation events (pl: moldboard plowing, mu: mulching). Arrows associated with uppercase letters followed by values indicate N inputs, including fertilization type (F: synthetic fertilizer, S: slurry, M: manure) and rates, in kg N ha^{-1}, respectively (e.g., M136 indicates a manure application at a rate of 136 kg N ha^{-1}). The crop growing periods from sowing to harvest or termination are indicated below the X-axis of the upper panels, empty spaces indicate non-growing periods. GM: green manure.

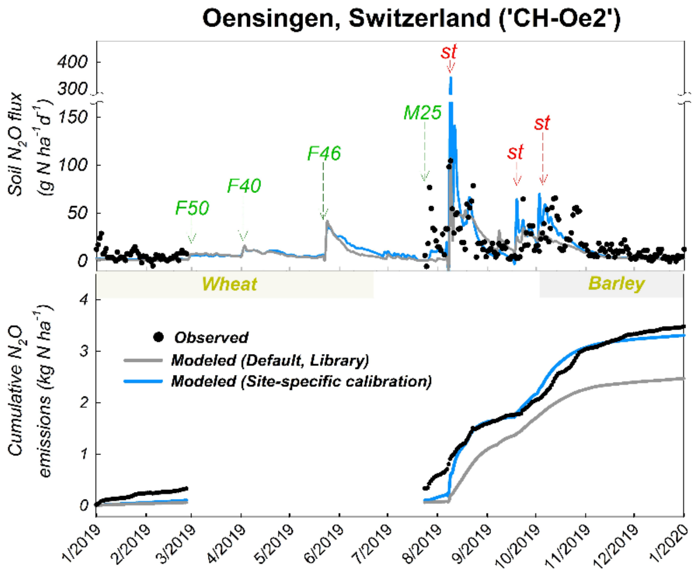

Figure 10: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the field study in Oensingen (Switzerland).
Arrows associated with lowercase letters indicate cultivation events (st: shallow tillage). Arrows associated with uppercase letters followed by values indicate N inputs, including fertilization type (F: synthetic N fertilizer or 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}). The crop growing periods from sowing to harvest are indicated below the X-axis of the upper panels; empty spaces indicate non-growing periods.

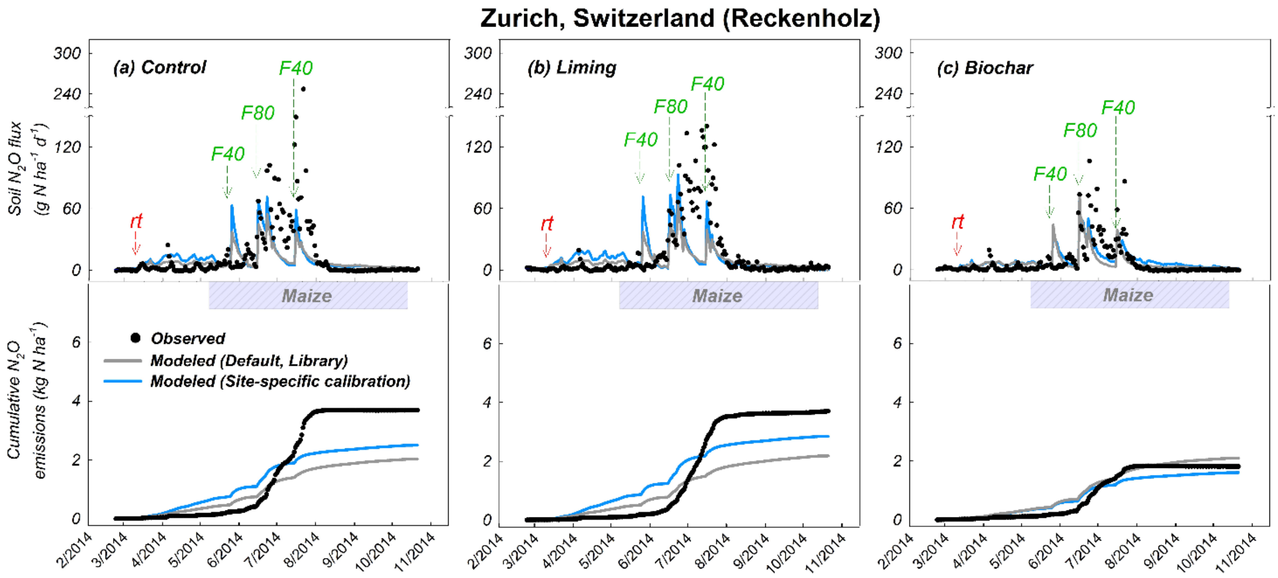

Figure 11: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the following treatments at Reckenholz in Zurich (Switzerland): 'Control' (a), 'Liming' (b) and 'Biochar' (c).
Arrows associated with lowercase letters indicate cultivation events (rt: rotary tillage). Arrows associated with uppercase letters followed by values indicate N inputs as synthetic fertilizer, in kg N ha^{-1} (e.g., F40 indicates an application of synthetic fertilizer at a rate of 40 kg N ha^{-1}). The maize growing period from sowing to harvest are indicated below the X-axis of the upper panels; empty spaces indicate non-growing periods

8.2 Model evaluation

Regressions of modeled against observed crop yields and N_2O emissions from crop cycles at the six sites were used to assess the performance of DayCent (*Figures 12* and *13*). They allowed to quantify the improvement in the estimates of crop yields and N_2O emissions by site-specific calibration (*Figures 12b* and *13b*) compared to the use of default parameters (*Figures 12*a and *13a*). Site-specific calibration increased the R^2 values from 0.43 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 48 to 29 % for crop yields and from 88 to 54% for mean N_2O fluxes. The positive bias slightly decreased for crop yields (from 29 to 23 g C m^{-2}) and turned into a negative bias for N_2O emissions (from 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 (*Figure 12a* and *12c*), although it was, as expected, lower compared to site-specific calibration (*Figure 12b* and *Figure 12c*). 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 likely limited a 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 and for long timeseries. The LOO cross-evaluation for N_2O emissions showed an R^2 of 0.63, which was still higher than 0.51 obtained using the default parameters (*Figure 13a* and *Figure 13c*). 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 N_2O emissions in the LOO cross-evaluation was achieved by adjusting the model parameters controlling nitrification and denitrification (*Figure 14*). 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 predictive ability of the model for N_2O emissions (Appendix I, Figure A.1).

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 WFPS on denitrification (*wfpsdnitadj*). Other parameters ended by presenting LOO averages close to the default values, like the N_2:N_2O ratio adjustment coefficient (*N2N2Oadj*), even presenting site-specific values deviated significantly from the default value (*Figure 14*).

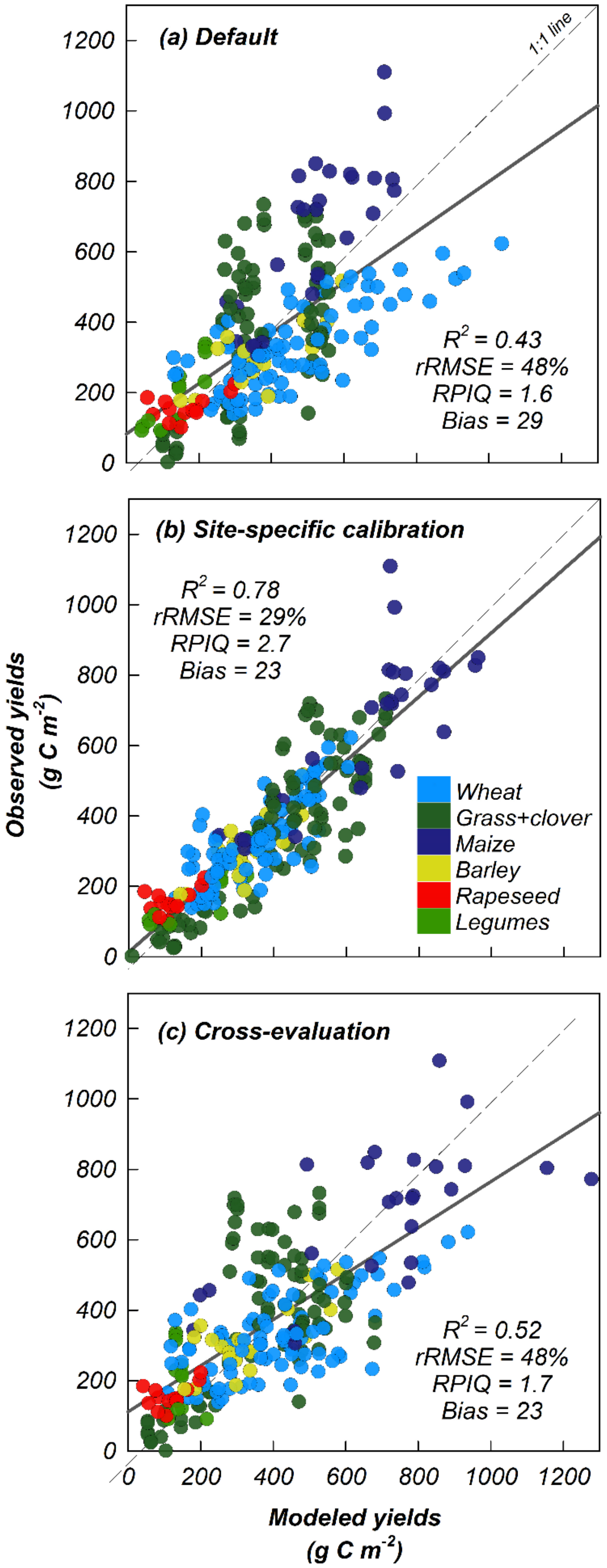

Figure 12: Modeled against observed crop yields for six different field studies in Switzerland and France. Model performance was assessed for default parameterization (a), site-specific calibration (b), and leave-one-out (LOO) cross-evaluation, i.e., the mean parameter value of all other sites except 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), the ratio of performance to interquartile distance (RPIQ) and the bias.

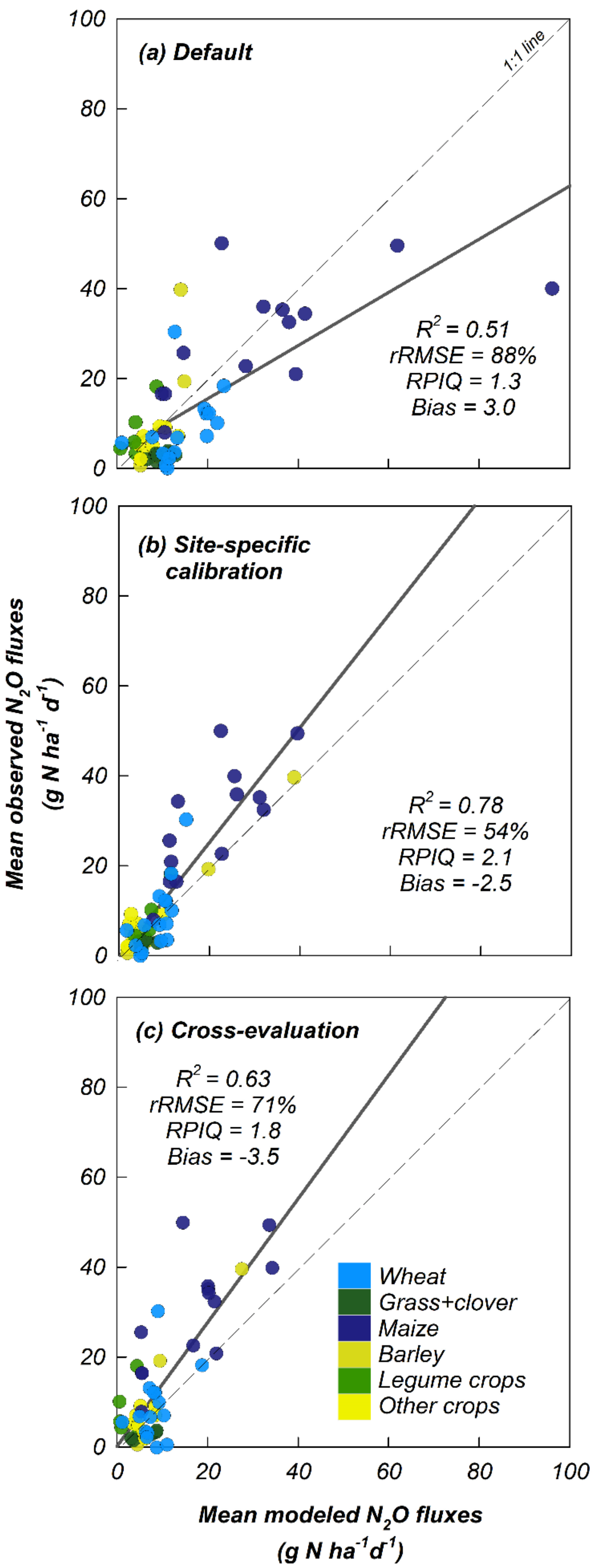

Figure 13: Mean modeled versus observed soil N_2O fluxes during different crop cycles of six sites in Switzerland and France.
Model performance was assessed for default parameterization (a), site-specific calibration (b), and leave-one-out (LOO) cross-evaluation, i.e., the mean parameter value of all 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 Figure 12. The error measures are explained in Figure 12.

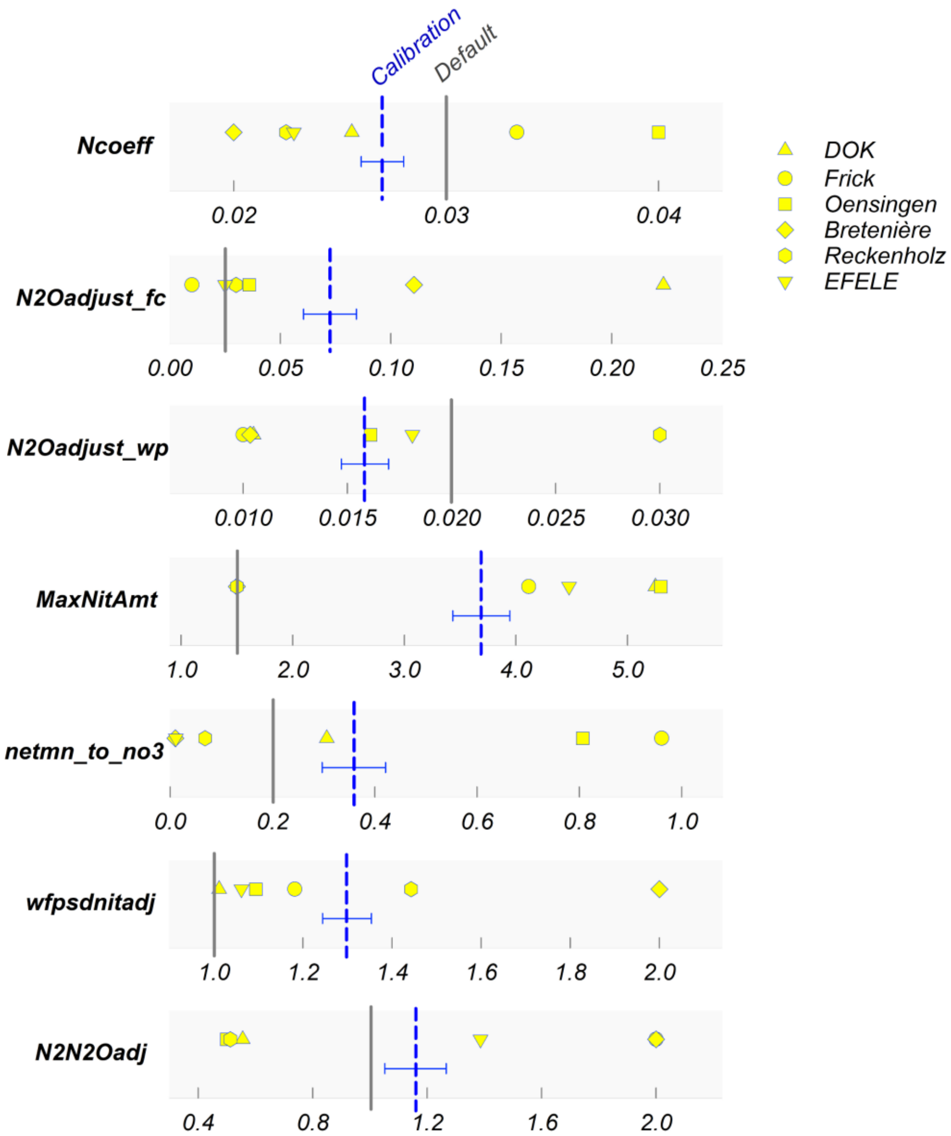

Figure 14: DayCent parameters controlling soil N_2O emissions before and after calibration based on data from six cropland field studies in Switzerland and France.
The grey solid vertical lines indicate the original default model values of the parameter, the dashed blue lines indicate the value of the average calibration using all six sites with horizontal blue bars indicating the confidence interval of the leave-one-out (LOO) values for α = 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 N_2O at field capacity, N2Oadjust_wp: minimum proportion of nitrified N lost as N_2O at wilting point, MaxNitAmt: maximum daily nitrification amount (g N m^{-2}), netmn_to_no3: fraction of new net mineralization that goes to NO_3^-, wfpsdnitadj: adjustment on inflection point for water-filled pore space (WFPS) effect on denitrification, N2N2Oadj: N_2:N_2O ratio adjustment coefficient.

For a comparison of modeled-based *vs.* EF approaches, we estimated the mean cumulated N_2O emissions for crop cycles with all management periods (N fertilization and tillage) covered by measurements with gap-filling, including winter (See *Section 6* above). 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 N_2O emissions for the selected crop cycles presented a wide range of values (0.7 to 7.0 kg N ha^{-1}) with a mean of 2.7 kg N ha^{-1} (*Figure 15*). Estimates based on EFs and model simulations with default parameterization were used in this project as "lower benchmarks" and estimates from models with site-specific calibration were used as "upper benchmarks". This means that the closer the model's performance is to the "lower benchmarks", the worse its predictive capacity, while the closer it is to the "higher benchmarks", the better the predictive ability. The N_2O emissions estimated using the aggregated EF approach, *i.e.*, considering 1% N losses from N inputs (Klein et al., 2007), presented a 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} (*Figure 15*). 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 to

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 (*Figure 15*). The mean model estimates with either site-specific calibration or LOO average of parameters were significantly better than the EF approaches. A central aspect to consider is that estimates based on EF do not explicitly account for the impact of tillage or the long-lasting effect of plant residues on the inter-seasonal variability of background N_2O emissions, which has been recognized as a major contribution to the total emission.

Although the model performs better than the EFs, the interquartile range of estimates is narrower, as indicated by the extent of bars. This indicates that the adjustment of model parameters by site-specific calibration or by applying LOO averages underestimates the highest and overestimates the lowest values of N_2O emissions per crop cycle.

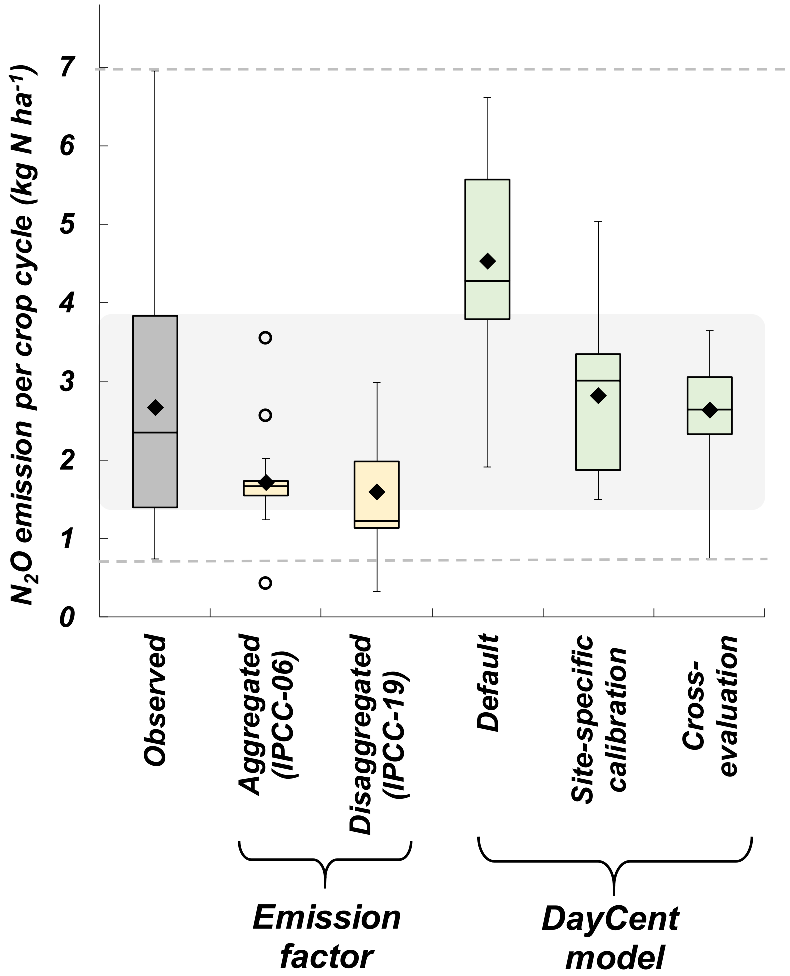

Figure 15: Box plots of cumulative N_2O emissions per crop cycle in field studies (n=23 crop cycles).

Different approaches were compared against observed N_2O emissions including IPCC emission factor (EF, yellow bars) and modeling (green bars). Estimates based on EF and model estimates with default parameters were used as “lower benchmarks”. Model estimates with site-specific calibration were used as “upper benchmark”. The range from the first to the third quartile are indicated by the length of the 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.

9 Performance of DayCent for grasslands

9.1 Site-specific calibration and simulation of daily N_2O fluxes

It revealed that plant parameters in DayCent with the largest relative changes compared to default values were those controlling N uptake, such as the thresholds of N sufficiency and deficiency and maximum BNF rates (*Table 6*, *Figure 16*). Adjusting these parameters resulted in an improvement of the model output with respect to the simulation of C and N yields and C:N ratio in the harvested biomass (*Figure 17*). The overestimation in the C:N ratio of more than 100% associated with the default parameters was consistently reduced in all sites and cuts after calibration (*Figure 17e-f*). Similarly, the overestimation in modeled N_2O emissions and N leaching was consistently reduced at all sites by model calibration (*Figures 18 to 22*). Additional improvements in simulated N loss were also obtained through calibration of soil parameters controlling N transformation in soil (*Figure 16*). For example, the ability of the model to simulate low N_2O fluxes under drier conditions depended on the calibration of the parameter '*N2Oadjust_wp*', which represents the minimum proportion of nitrified N lost as N_2O at the wilting point (*Figure 16*).

9.2 Model evaluation

Also for grassland, a cross-evaluation was performed to assess the predictive ability of the model, *i.e.,* to make out-of-sample predictions. In this case, parameter values were specified as the average of the parameter values for the complementary sites. Annual N_2O emissions and N leaching were used as indicators of the predictive ability of the model (*Figure 23*, *Table 7*). As "lower performance benchmarks" for out-of-sample predictions, we used (*i*) annual N_2O emissions and N leaching estimates computed based on the IPCC's EF approach[6] (Hergoualc'h et al., 2019) and (*ii*) the results of the uncalibrated model, *i.e.,* reflecting default parameter values (*Figure 23a-b*, *Figure 16*, *Table 7*). As "upper benchmark" we used the model estimates with site-specific calibration.

All statistical metrics (*R^2, rRMSE, RPIQ, and bias*) in the cross-evaluation for N_2O emissions show that, overall, the performance of the model for out-of-sample conditions, *i.e.,* shown in the cross-evaluation, is much closer to the upper benchmark represented by site-specific calibration, than to the lower benchmarks represented by the EF approach and default parameterization (*Figure 23*). For N leaching, the improvement was more evident considering the *bias* and *rRMSE* values even though the R^2 values did not discriminate very well between the different approaches (*Table 7*, *Figure 24*). This result indicates that DayCent is a suitable tool for simulating grassland ecosystem processes at the local scale even if only representative parameter values for the regional scale are available.

[6] For grasslands, we are presenting only the disaggregated EF approach as "lower benchmark". Estimates using aggregated EF did not present significant differences in comparison to disaggregated EF (results not shown).

Table 6: Description of calibrated parameters for permanent grassland sites in Western Europe.

Parameter	**Description**	**Reference**
prdx(1) [1]	Coefficient for calculating potential production as a function of solar radiation (g C m^{-2} $month^{-1}$ $Langley^{-1}$)	Necpalova et al. (2018), Gaillard et al. (2018)
ppdf(1) [2]	Optimum temperature for growth (°C)	Necpalova et al. (2018)
pramn(1,1)	Minimum aboveground C/N ratio in the beginning of the growth curve	Necpalova et al. (2018)
pramn(1,2)	Minimum aboveground C/N ratio with biomass > biomax	Necpalova et al. (2018)
pramx(1,1)	Maximum aboveground C/N ratio in the beginning of the growth curve	Necpalova et al. (2018)
pramx(1,2)	Maximum aboveground C/N ratio with biomass > biomax	Necpalova et al. (2018)
biomax	Biomass above which *pramn(1,2)* and *pramx(1,2)* equal the minimum and maximum C/N ratios of the new growth respectively (g biomass m^{-2})	Necpalova et al. (2018)
snfxmx(1)	Maximum BNF [3] [g N_2 fixed (g C new $biomass)^{-1}$]	Necpalova et al. (2018)
Ncoeff	Minimum water and temperature limitation coefficient for nitrification	Martins et al. (2022)
N2Oadjust_fc	Maximum proportion of nitrified N lost as N_2O at field capacity	Gaillard et al. (2018), Martins et al. (2022)
N2Oadjust_wp	Minimum proportion of nitrified N lost as N_2O at wilting point	Gaillard et al. (2018), Martins et al. (2022), Hong et al. (2023)
netmn_to_no3	Fraction of new net mineralization that goes to NO_3^-	Gaillard et al. (2018), (Martins et al., 2022), Hong et al. (2023)
wfpsdnitadj	Adjustment on inflection point for WFPS [4] effect on denitrification	Gaillard et al. (2018), Martins et al. (2022), Hong et al. (2023)
N2N2Oadj	N_2:N_2O ratio adjustment coefficient	Gaillard et al. (2018), Martins et al. (2022), Hong et al. (2023)

[1] It reflects the genetic potential of the plants;
[2] this parameter defines the Poisson density function curve to simulate the temperature effect on plant growth;
[3] BNF: biological N_2 fixation.
[4] WFPS: water-filled pore space.

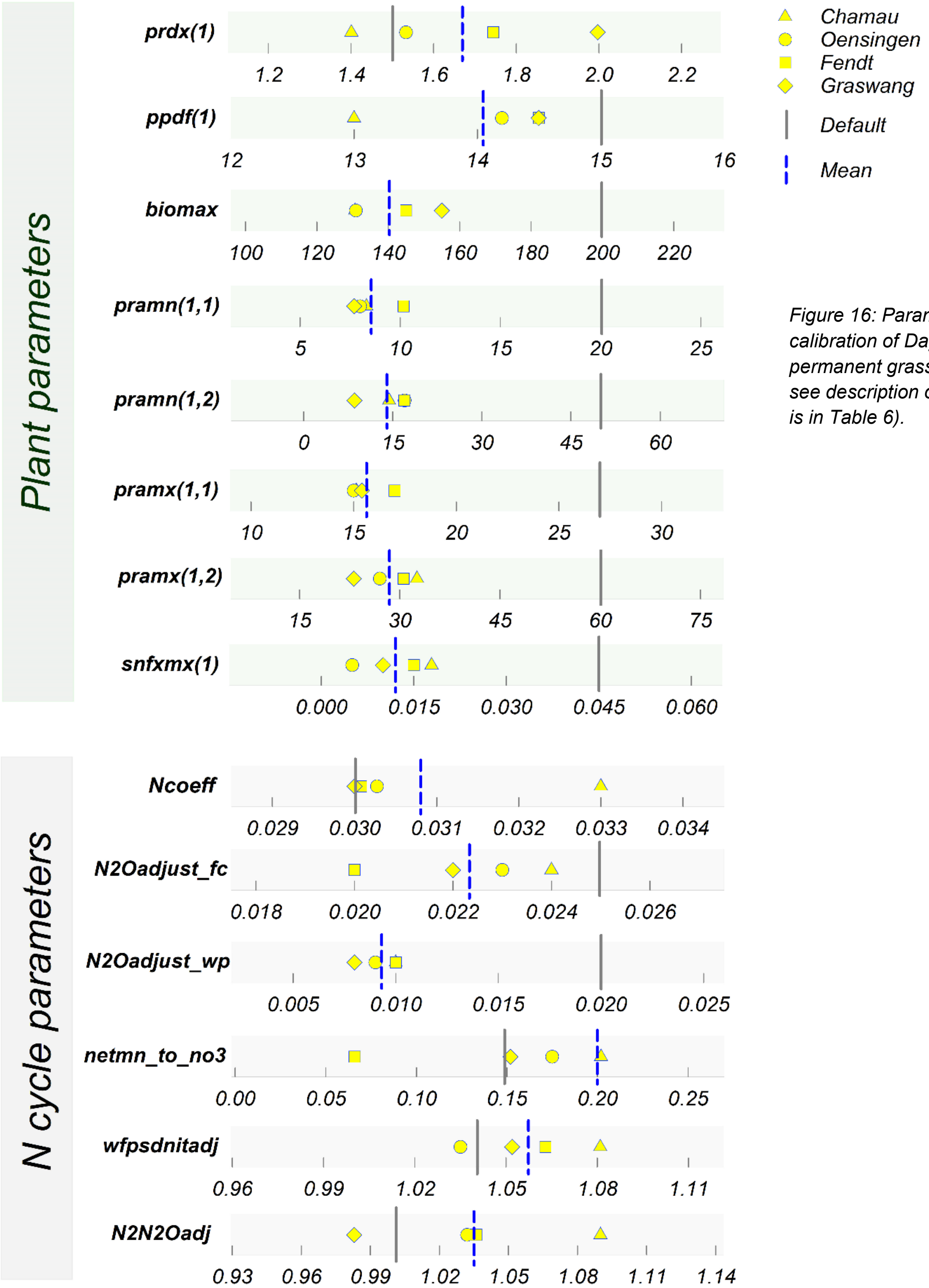

Figure 16: Parameter values after calibration of DayCent for permanent grassland sites (please see description of the parameters is in Table 6).

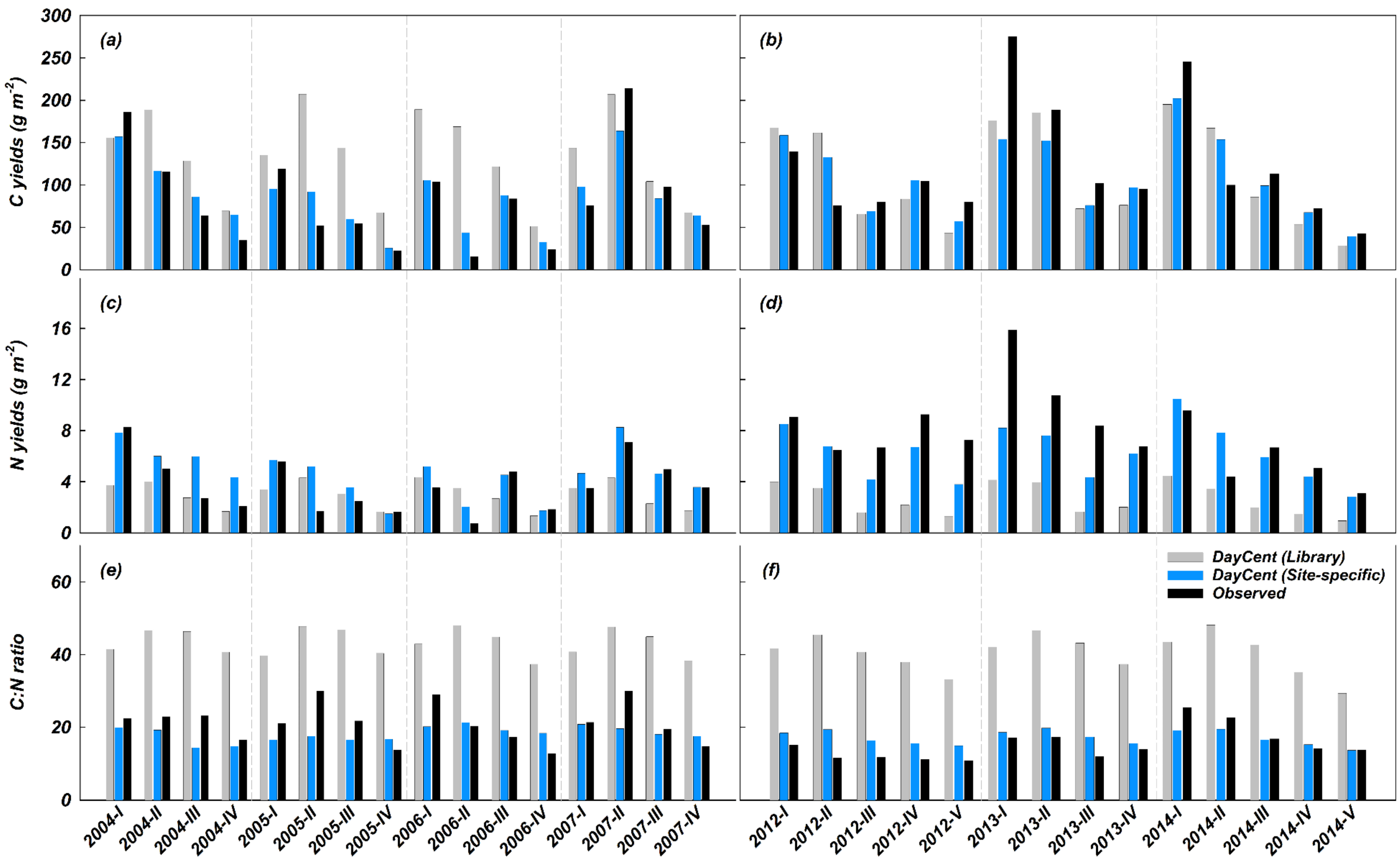

Figure 17: Modeled against observed C and N yields and C:N ratios in sequential mowing events in grasslands under intensive treatment at Oensingen, Switzerland (a, c and e) and Fendt, Germany (b, d and f). The results for these two sites are used as an example to show the basic performance of the model to simulate plant growth and N uptake before and after model calibration.

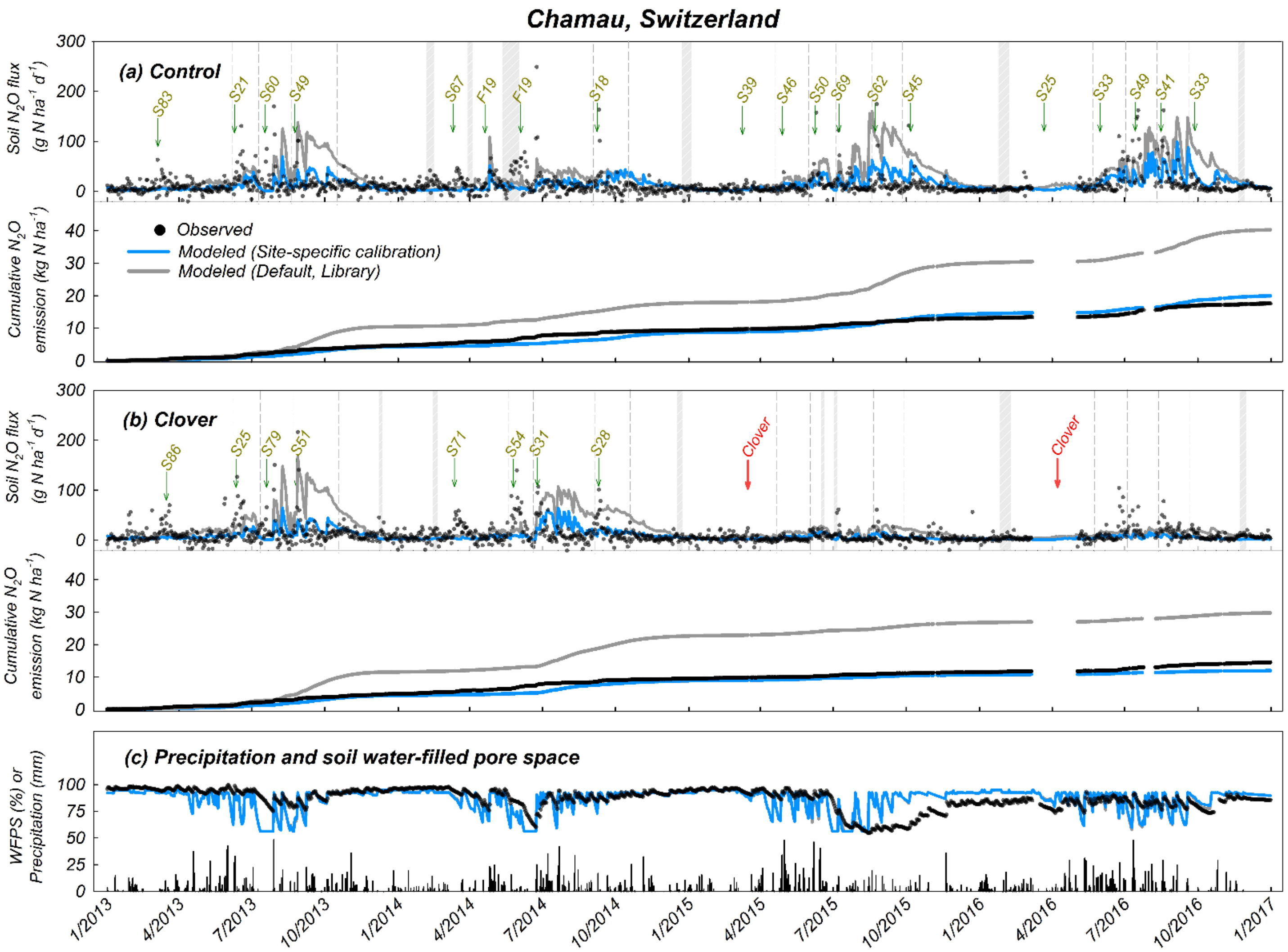

Figure 18: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the grassland site in Chamau, Switzerland, under 'control' (a) and 'clover' (b) managements. Vertical dashed lines indicate harvest events. Grazing periods are denoted by gray-shaded areas. Arrows associated with uppercase letters followed by values indicate N inputs, in kg N ha^{-1}, as synthetic fertilizer (F) or slurry (S). For example, 'S83' indicates an application of slurry at a rate of 83 kg N ha^{-1}. The arrows associated with "Clover" indicate the oversowing of clover in the plots. The last Figure (c) shows the precipitation (black bars) and the soil water-filled pore space (WFPS) averaged between the two plots.

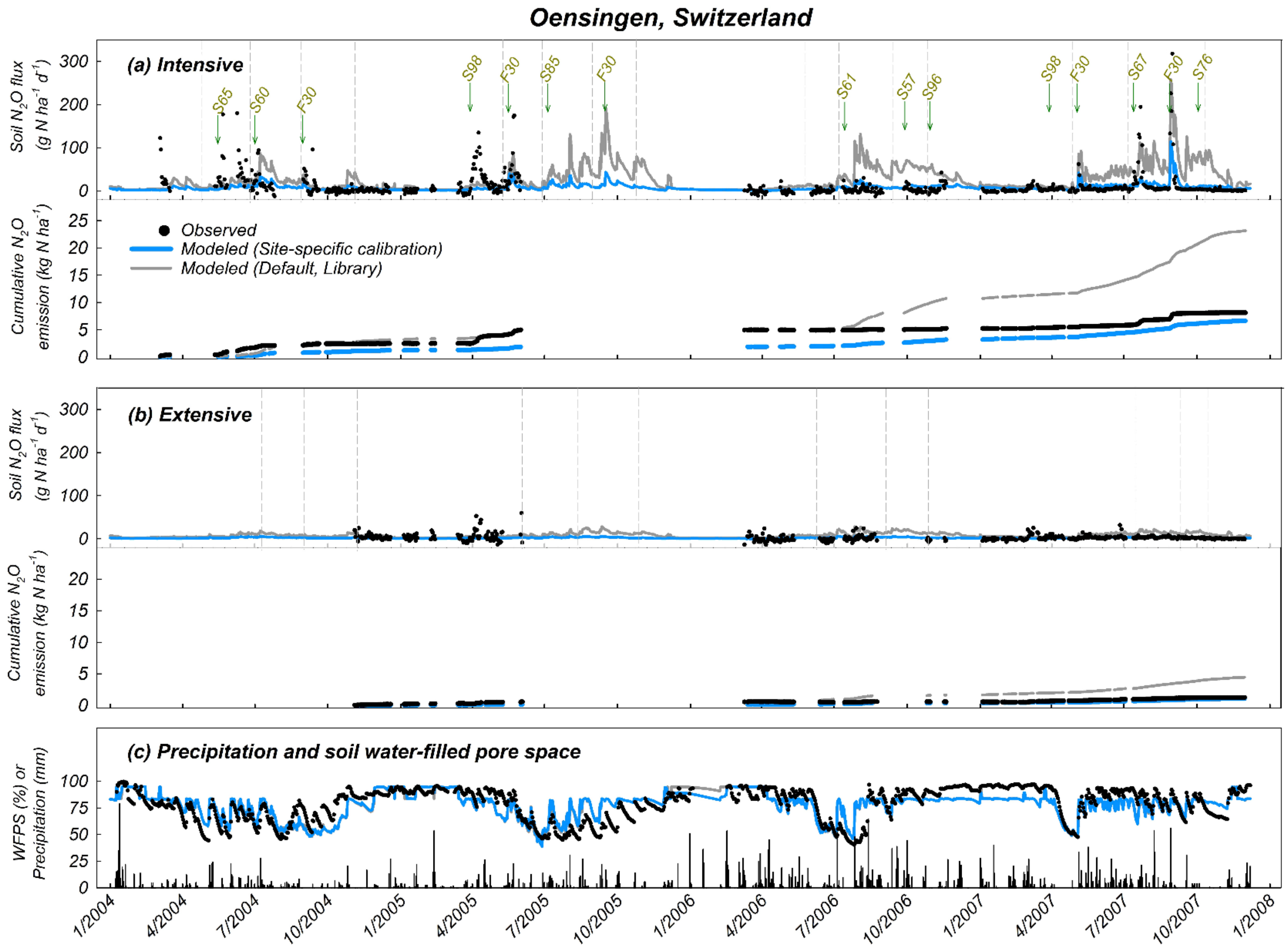

Figure 19: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the grassland site in Oensingen, Switzerland, under 'intensive' (a) and 'extensive' (b) managements. Vertical dashed lines indicate harvest events. Arrows associated with uppercase letters followed by values indicate N inputs, in kg N ha^{-1}, as synthetic fertilizer (F) or slurry (S). For example, 'S65' indicates an application of slurry at a rate of 65 kg N ha^{-1}. The last Figure (c) shows the precipitation (black bars) and the soil water-filled pore space (WFPS) averaged between the two plots.

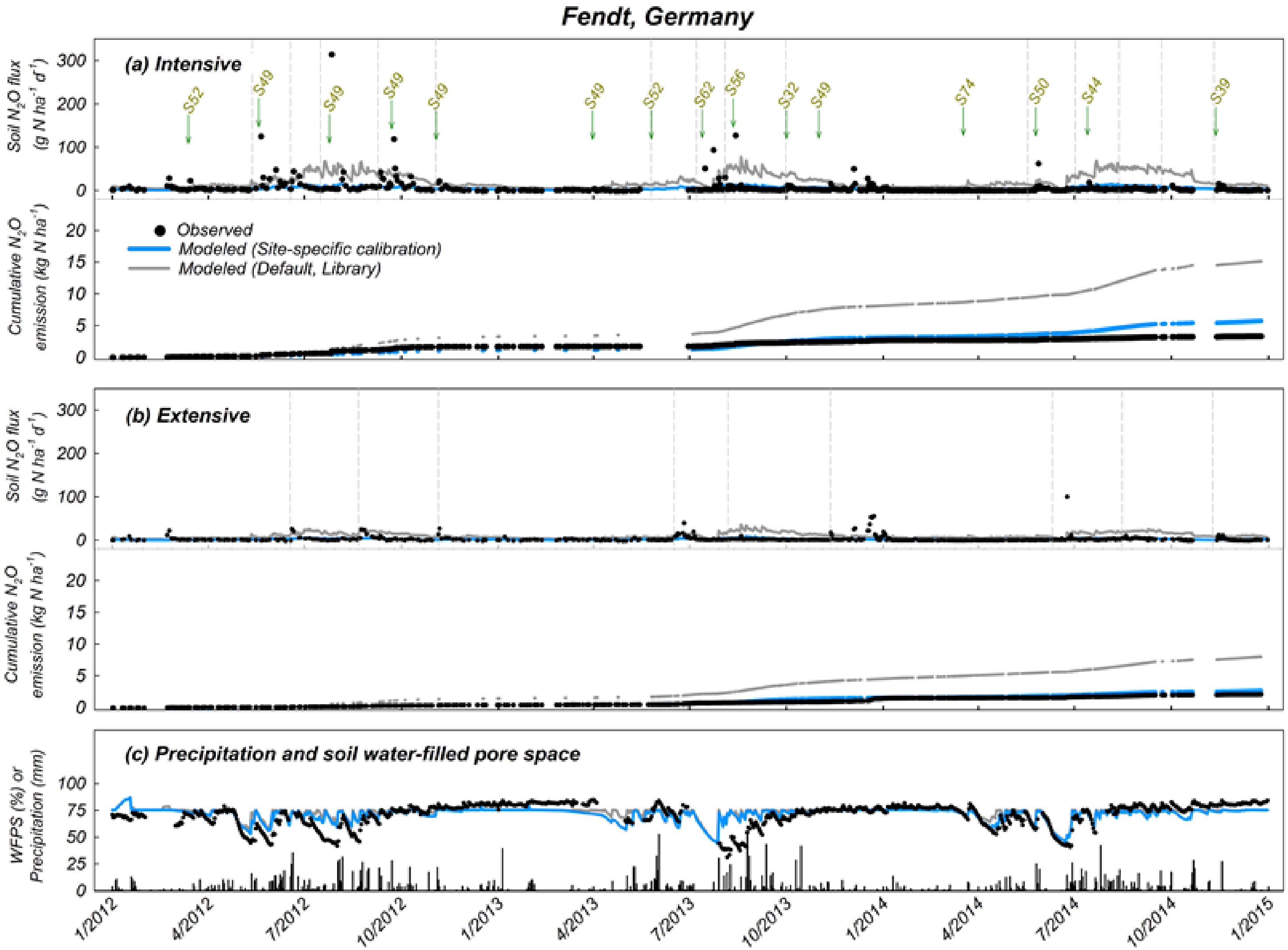

Figure 20: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the grassland site in Fendt, Germany, under 'intensive' (a) and 'extensive' (b) managements.
Vertical dashed lines indicate harvest events. Arrows associated with uppercase letters followed by values indicate N inputs, in kg N ha^{-1}, as synthetic fertilizer (F) or slurry (S). For example, 'S52' indicates an application of slurry at a rate of 52 kg N ha^{-1}. The last Figure (c) shows the precipitation (black bars) and the soil water-filled pore space (WFPS) averaged between the two plots.

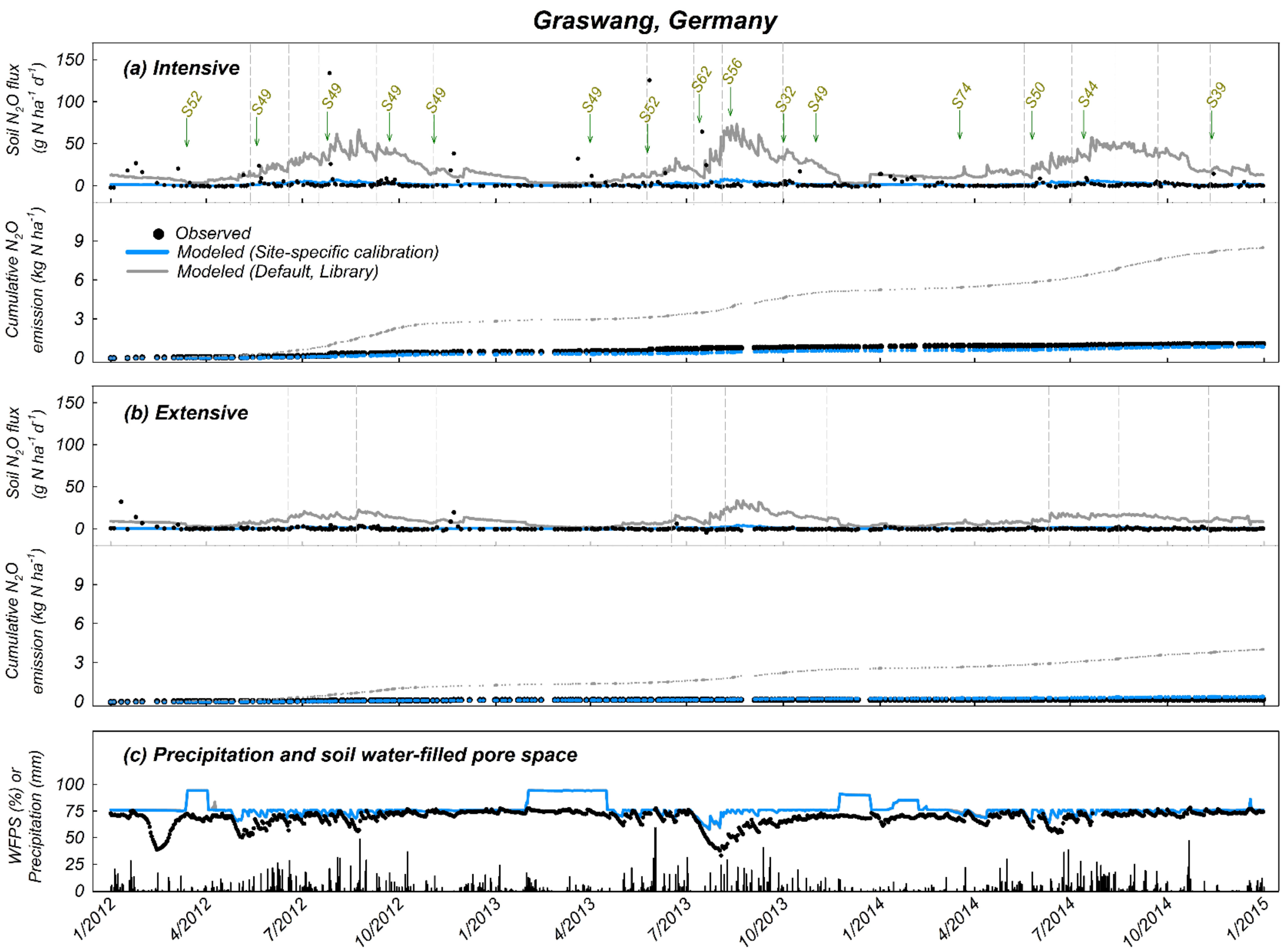

Figure 21: Modeled (lines) versus observed (symbols) daily soil N_2O fluxes (top panels) and cumulative N_2O emissions (lower panels) from the grassland site in Graswang, Germany, under 'intensive' (a) and 'extensive' (b) managements. Vertical dashed lines indicate harvest events. Arrows associated with uppercase letters followed by values indicate N inputs, in kg N ha^{-1}, as synthetic fertilizer (F) or slurry (S). For example, 'S52' indicates an application of slurry at a rate of 52 kg N ha^{-1}. The last Figure (c) shows the precipitation (black bars) and the soil water-filled pore space (WFPS) averaged between the two plots.

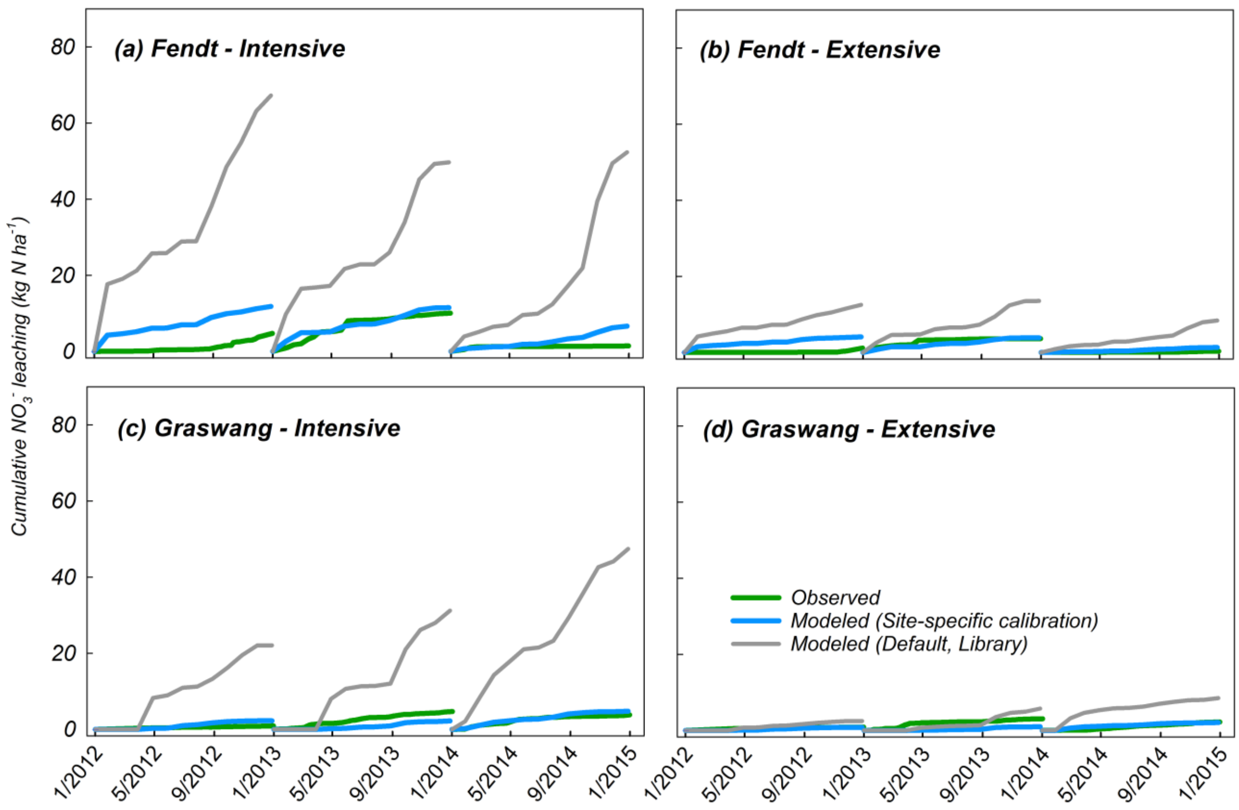

Figure 22: Modeled and observed annual cumulative nitrate leaching losses from grassland sites under different management intensities.

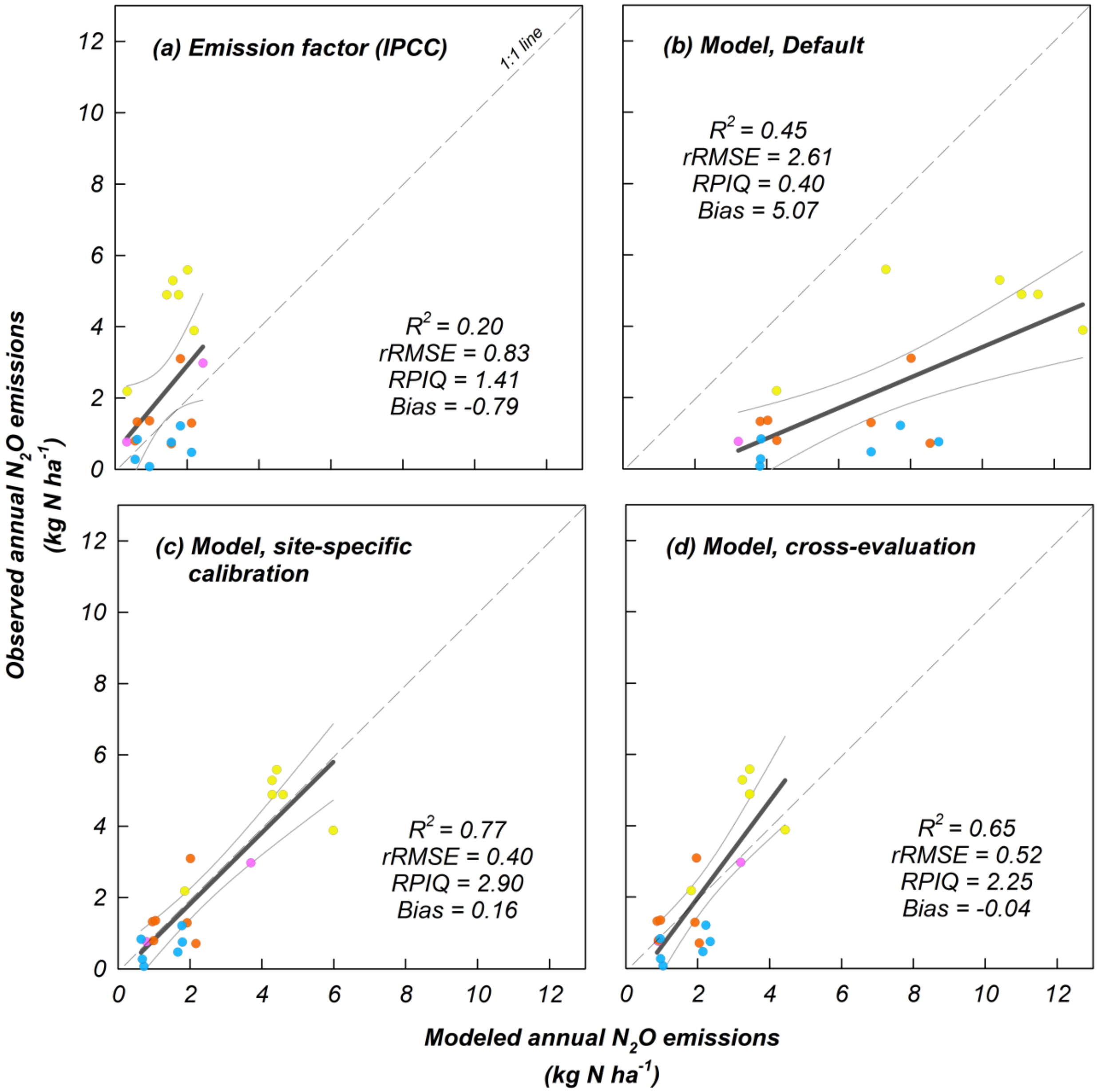

Figure 23: Modeled against observed annual N_2O emissions of grassland sites under different management types over multiple years. The emissions from different sites are displayed by different colors of symbols: yellow, Chamau; pink, Oensingen; orange, Fendt; blue, Graswang.
Estimates based on emission factors indicated by IPCC (Hergoualc'h et al., 2019) (a) and model estimates with default parameters (b) were used as "lower benchmarks". Model estimates with site-specific calibration were used as "upper benchmark" (c). The cross-evaluation of the model (d) was based on the use of LOO average of parameters, i.e., an average from calibrated parameters from all the sites, except the one being evaluated. Dark grey lines indicate the trend of linear adjustment and light grey lines the associated 95% confidence interval. The dashed identity lines indicate the potential perfect adjustment of the modeled to the observed values. The coefficient of determination (R^2), the relative root mean square error (rRMSE), the ratio of performance to interquartile distance (RPIQ) and the bias, in kg $N\text{-}N_2O\ ha^{-1}\ yr^{-1}$, were used to measure the agreement between modeled and observed emissions.

Table 7: Performance of DayCent and IPCC's EF approach for estimating N leaching at two grassland sites in Germany; the coefficient of determination (R^2), the relative root mean square error (*rRMSE*), the ratio of performance to interquartile distance (*RPIQ*) and *bias* were used to measure the agreement between modeled and observed emissions.

Prediction approach [1]	***Mean*** **(kg N ha^{-1})**	R^2	***rRMSE***	***RPIQ***	***Bias*** **(kg N ha^{-1})**
Emission factor (IPCC)	37.9	0.42	8.30	0.08	33.1
Model, default	27.7	0.23	6.36	0.11	22.9
Model, site-specific	5.0	0.45	0.58	1.19	0.2
Model, cross-evaluation	5.4	0.42	0.62	1.11	0.6
Observation	4.8	-	-	-	-

[1] Estimates based on emission factor (EF) indicated by IPCC (Hergoualc'h et al., 2019) and model estimates with default parameters were used as "lower benchmarks". Model estimates with site-specific calibration were used as "upper benchmark". The cross-evaluation of the model was based on the use of LOO average of parameters, *i.e.,* an average from calibrated parameters from all the sites, except the one being evaluated.

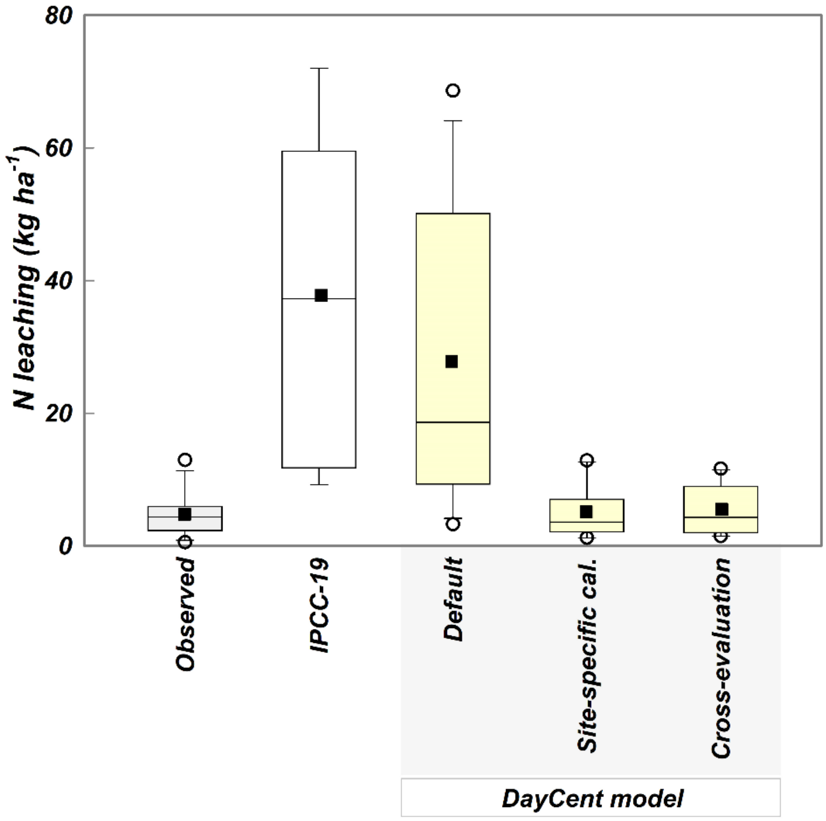

Figure 24: Box plots of the annual N leaching based on observed and estimated values for two grassland sites in Germany. The EF approach (referred to as IPCC-19) considers a default value of 24% of N losses as leaching in regions with precipitation exceeding evapotranspiration (Hergoualc'h et al., 2019), which is the case for sites in the present study. The EF approach was used in the present study as a "benchmark" for comparison with DayCent model performance. The length of the boxes represents the distance from the first to the third quartile. The median values of N leaching losses are indicated by horizontal lines within the boxes and square symbols indicate mean values. Whiskers represents the upper and lower extremes and circles represents the outliers.

10 Regional simulations

The next step after calibration and evaluation of the model based on field measurement data was to carry out a first upscaling of model-based estimates of N_2O emissions. The main purpose was to set up a system, that can later be used for national-scale modelling. In this first upscaling, an oversimplified approach was considered for the management information (*i.e.*, no spatial difference in fertilization rates or crops grown) due to a lack of information. However, in the case of soil, weather and land-use data, more information is available. This geospatial data was gathered and processed to be used as input data for modelling. This is a crucial step for model simulations on a regional scale. Various R functions were used to pre- and post-process simulation data. Specific R packages for processing geospatial data (raster and vector) were used, such as '*terra*', '*sf*', '*sp*', and '*spLarge*'. The integrated development environment RStudio (Campbell, 2019) was used to develop a script to run DayCent and to obtain figures and data outputs of regional simulations.

For this last phase of the project, we partly use the same procedures applied for simulations of SOC stocks in agricultural soils for the national GHG emissions inventory which apply the model RothC (Wüst-Galley et al., 2019). One advantage of using an approach partially similar to the one already adopted for SOC is that it can provide a more consistent GHG reporting in the future. In the present project, the model simulations were performed considering the period from 1990 to 2021.

10.1 Definition of strata for regional simulations

The first approach for the regional simulations of N_2O emissions was based on stratification of the Swiss territory. The splitting in strata followed a similar procedure used for modeling SOC stocks (Wüst-Galley et al., 2019). It was based on the combination of two types of geospatial data. Firstly, four agricultural zones defined by the Federal Office of Agriculture (FOAG, 2020) were considered:

- ***A1: Valley region***
- ***A2: Hill region***
- ***A3: Mountain region***
- ***A4: Summer pasture region***

A main reason of using the agricultural zones in our project is that management practices are considered to be relatively homogenous inside each unit. In a second step, five production regions from the national forest inventory (NFI), obtained from the Swiss Federal Institute for Forest, Snow and Landscape Research (WSL, 2023), were used to perform a further splitting of the agricultural land that mainly considers differences in climatic conditions and are defined as follows:

- ***F1: Jura***
- ***F2: Central Plateau***
- ***F3: Pre-alps***
- ***F4: Alps***
- ***F5: Southern Alps***

This splitting in five regions is already been used in the Land Use, Land-Use Change and Forestry (LULUCF) sector. The combination of agricultural zones and production zones produced 20 strata.

After this initial stratification from the combination of agricultural zones and production regions (A1_F1, A1_F2 etc.), some larger strata presenting potential variability of climatic conditions that were not accounted for, were further subdivided according to climate regions defined by MeteoSwiss (Schüepp and Gensler, 1980). The applied to the alpine region (strata from the F4 region) that was subdivided in western (suffix W) and central (suffix C) subregions, resulting in eight strata instead of four delineated only by different production regions. Besides this, the stratum A1_F2, which represents about two thirds of the cropland area, was subdivided into three new strata representing western, central and eastern subregions (suffixes W, C and E, respectively), also according to the climate regions of MeteoSwiss. These subdivisions created a total of 26 strata, which were used in this project (*Figure 25*).

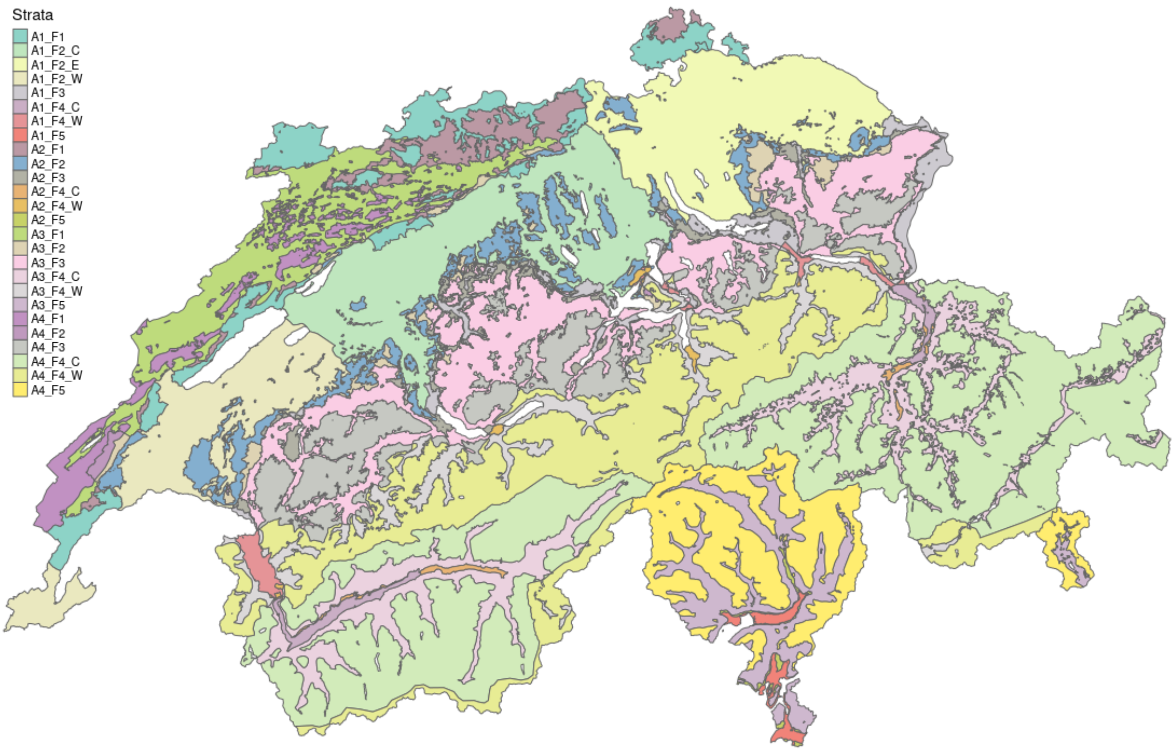

Figure 25: Stratification of the Swiss territory used in the LACHSIM project for regional DayCent simulations of N_2O emissions.

10.2 Land use data

The statistics of land use in Switzerland generated by the Swiss Federal Statistical Office (FSO) was used to define the location of cropland and grassland areas. The land use statistics for the year 2021 was used in this first upscaling of model simulations and extrapolated to the entire period of simulation. The N_2O simulations were performed for the combination categories defined as croplands (CC21) and grasslands (CC31). These categories are consistent with the nomenclature that has been used in the Swiss greenhouse gas inventory (FOEN, 2023; Wüst-Galley et al., 2019). Grass-clover leys were considered as part of croplands because they are not permanent and are typical elements of Swiss crop rotations. For permanent grassland following subcategories were distinguished in the simulations: intensive meadows, semi-intensive meadows, extensive meadows, intensive pastures, extensive pastures and summer pasture.

10.3 Weather data

DayCent simulations require daily weather data for precipitation, air temperature (maximum and minimum), solar radiation, relative humidity and wind speed (*Section* ***Fehler! Verweisquelle konnte nicht gefunden werden.***). In the present project different meteorological data sources were compared to SOC modelling based on RothC. For the latter gridded data were averaged for each stratum to represent monthly sums of precipitation and averages of air temperature and evapotranspiration (Wüst-Galley et al., 2019). This approach would not be suitable for N_2O simulations with DayCent, considering the high co-variability of N_2O with weather variables, especially in the case of precipitation. Furthermore, averaging daily data across grid points/measurement stations to represent values for a stratum would create an erroneous distribution of precipitation over time, likely eliminating temporal hotspots of N_2O emissions. Therefore, in this first explorative approach for upscaling N_2O emissions, we used daily data from one representative meteorological station per stratum (*Figure 26*). In the future, digital maps of daily weather data produced by MeteoSwiss with fine resolution could be applied for further improvements of the regional simulations of N_2O emissions.

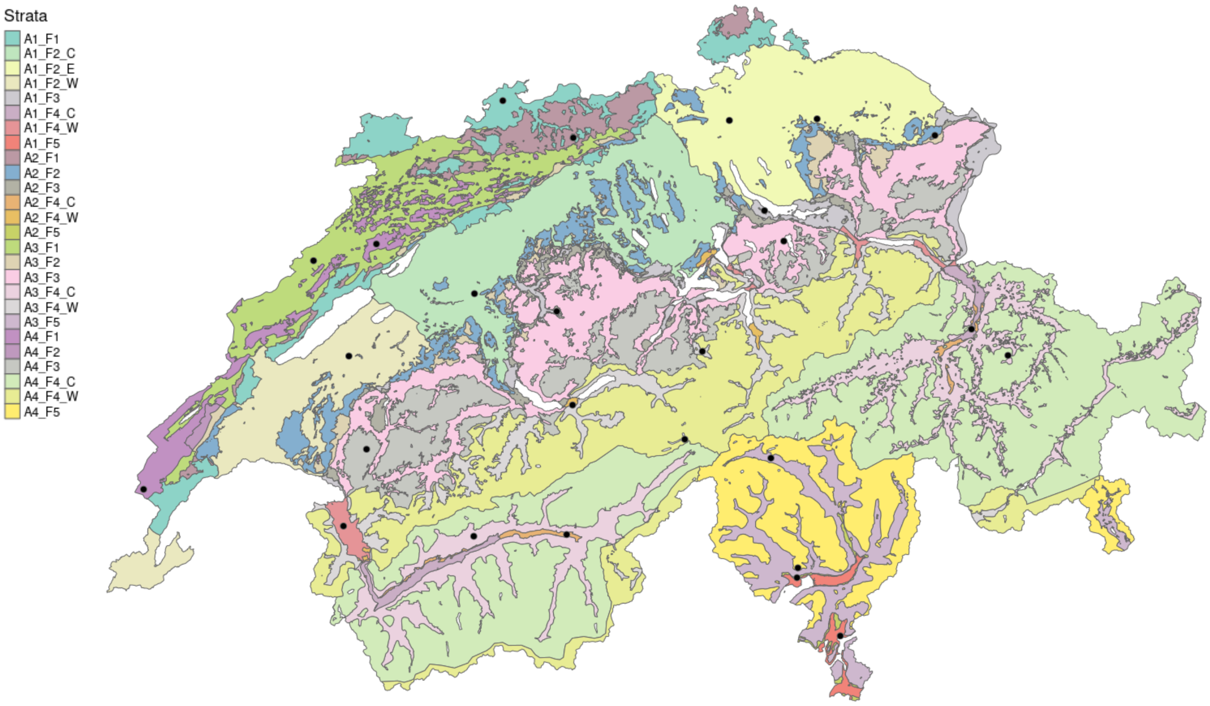

Figure 26: Weather stations (black dots) considered in the present project to obtain weather daily data as inputs for DayCent simulations of N_2O emissions.

10.4 Soil data

To carry out N_2O emission simulations, DayCent requires data on different soil physical and chemical properties and also on soil layer structure. All the soil properties and data sources for the regional simulations of N_2O emissions are presented in *Table 8*. A primary source of soil data were digital maps produced by the National Competence Center for Soil ("*Kompetenzzentrum Boden*", acronym KOBO). Digital maps of pH and contents of clay, sand and organic C, represented on a 30-m resolution raster, were provided by KOBO. These maps were generated using machine learning modeling, specifically with "Quantile Regression Forest" (Stumpf et al., 2021). The machine learning design was based on extensive field measurements of basic soil properties across the Swiss territory, including not only the properties being predicted (pH, SOC, clay and sand content), but also other co-variables describing terrain, climate, vegetation, land use and lithology of Switzerland (Stumpf et al., 2021).

Table 8: Soil properties used as DayCent inputs for the regional simulations of N_2O emissions.

Soil property	Unit	Data source for regional simulations
Sand fraction [1]	g g^{-1}	Map of soil texture from KOBO (Stumpf et al., 2021)
Clay fraction [1]	g g^{-1}	Map of soil texture from KOBO (Stumpf et al., 2021)
Silt fraction [1]	g g^{-1}	Obtained by subtraction (Silt = 1.0 – sand – clay)
Organic fraction [2]	g g^{-1}	Map of SOC contents from KOBO (Stumpf et al., 2021)
BD [3]	g cm^{-3}	Estimated using the PTF [8] described by Wösten et al. (1999); variables of the function are land use (whether land is cultivated or not) and contents of SOC, sand and clay (Stumpf et al., 2021)
Field capacity [4]	cm^3 cm^{-3}	Estimated using the PTF described by Saxton and Rawls (2006); using BD and contents of SOC, sand and clay (Stumpf et al., 2021)
Wilting point [4]	cm^3 cm^{-3}	Estimated using the PTF described by Saxton and Rawls (2006) using BD and contents of SOC, sand and clay (Stumpf et al., 2021)
Fraction of roots [5]	-	Default values provided by DayCent developers (Hartmann et al., 2019)
Δ_{min} [6]	cm^3 cm^{-3}	Default values provided by DayCent developers (Hartmann et al., 2019)
K_{sat} [7]	cm s^{-1}	Estimated using the PTF described by Saxton and Rawls (2006); the variables of the function are BD, field capacity and wilting point described above and sand, clay and SOC contents (Stumpf et al. 2021).
pH	-	Map of soil pH from KOBO (Stumpf et al. 2021)

[1] The values correspond to proportion in the mineral fraction (clay + silt + sand = 1.0).
[2] Used only for simulation of soil temperature, *i.e.,* not directly for simulating dynamics of soil organic pools and soil organic C (SOC) stocks.
[3] Bulk density.
[4] These are considered to be critical points for estimating soil water availability for plant growth.
[5] Fraction of roots in soil layer (sum of fractions from different layers = 1.0)
[6] The maximum amount of the volumetric soil water content that can be lost below wilting point – it is used to estimate the minimum achievable water content in the soil (minimum soil water content = wilting point – Δ_{min}).
[7] Saturated hydraulic conductivity.
[8] PTF: Pedotransfer function.

Based on contents of clay, sand and SOC, we applied PTFs to estimate soil BD, field capacity, permanent wilting point and K_{sat} to be used as model inputs. The PTFs used for this purpose are listed in *Table 8*. The maps produced using PTFs are presented below for BD (*Figure 27*), field capacity (*Figure 28*), permanent wilting point (*Figure 29*), and K_{sat} (*Figure 30*). In addition to being used as model inputs and for estimating other physical properties, the clay and sand data were also used to classify the soil texture into 12 classes (*Figure 31*). The classification of soil texture were performed using the R package '*soiltexture*' (Moeys et al., 2022).

In addition to the soil data described above, information on soil thickness had to be gathered/prepared as it is required as an input for DayCent. Geospatial data of soil thickness classes were obtained from the Swiss Soil Suitability Map (Häberli, 1980), which is used to classify surfaces according to their suitability for agriculture and forestry. A digital vector version of this map was available from the Federal Statistical Office (FSO, 2000).

Figure 27: Map of soil bulk density (BD), in g cm^{-3}, estimated using a pedotransfer function (PTF) described by Wösten et al. (1999); the dependent variables of the function are land use (whether the soil is cultivated or not) and contents of soil organic C (SOC), sand and clay.

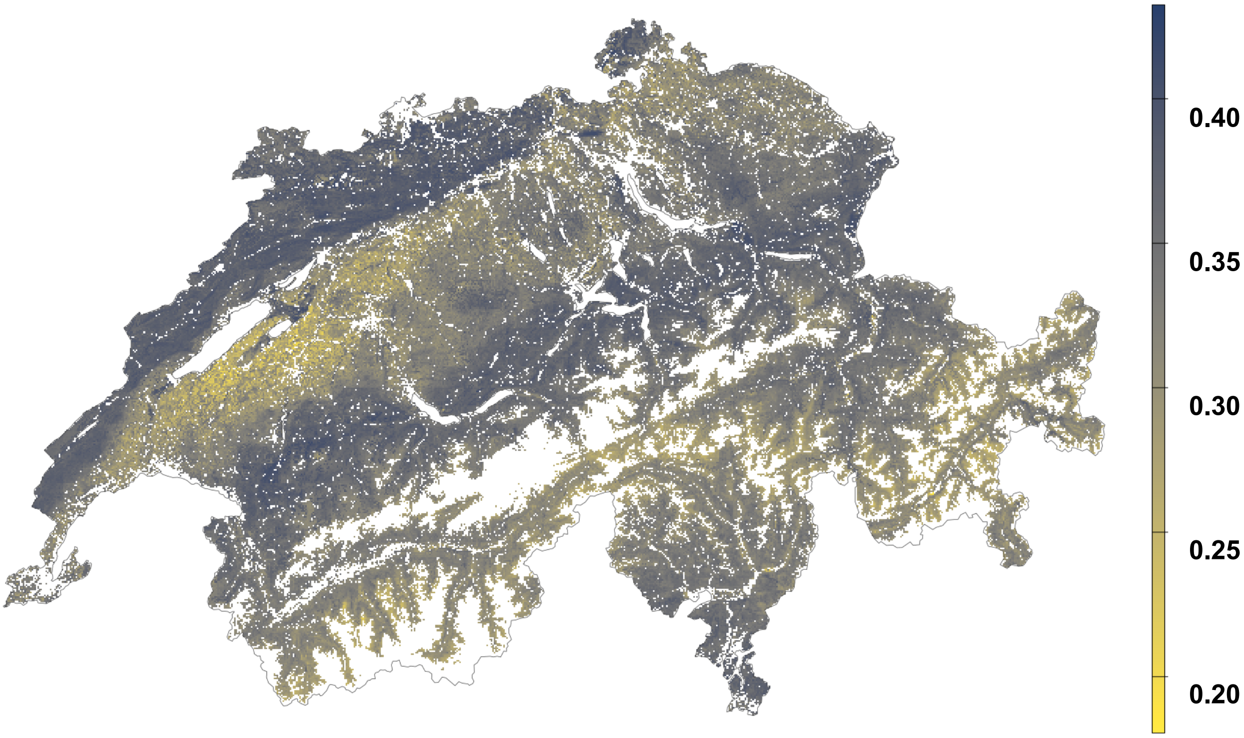

Figure 28: Map of soil water content at field capacity, in cm^3 cm^{-3}, estimated using a pedotransfer function (PTF) described by Saxton and Rawls (2006); the dependent variables of the function are bulk density (BD) and contents of soil organic C (SOC), sand and clay.

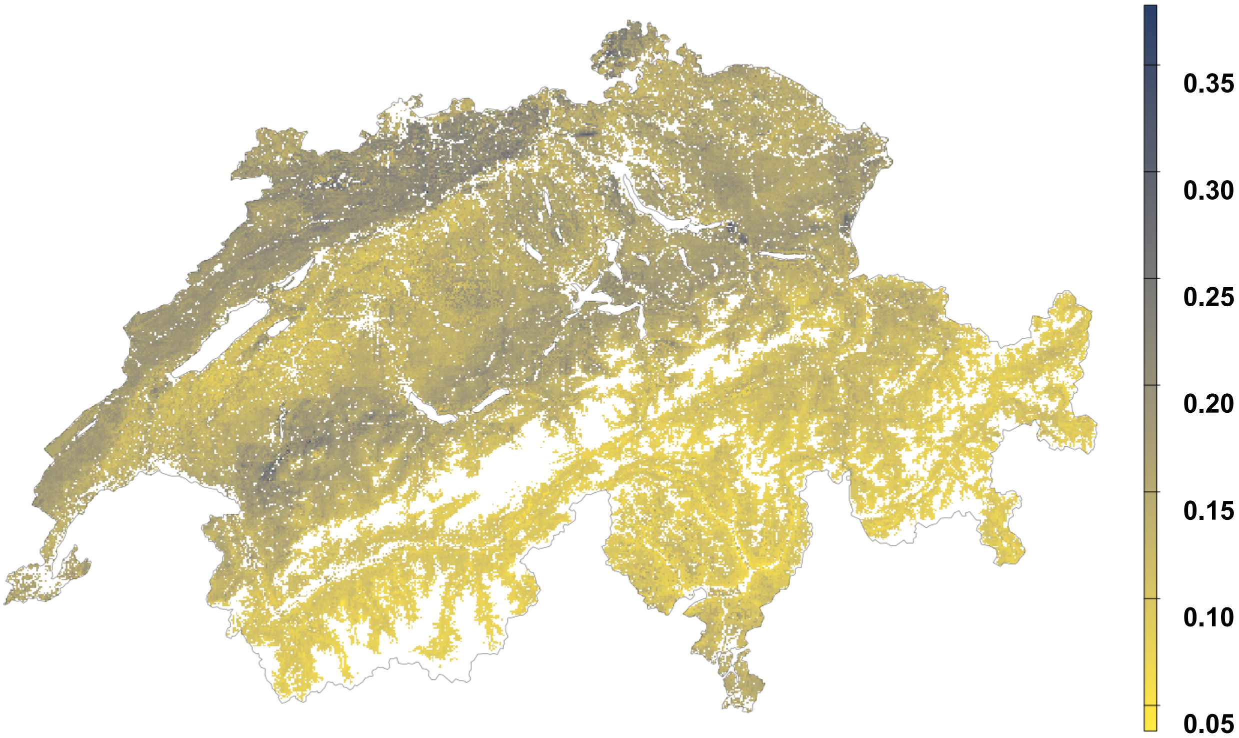

Figure 29: Map of soil water content at permanent wilting point, in cm^3 cm^{-3}, estimated using a pedotransfer function (PTF) described by Saxton and Rawls (2006); the dependent variables of the function are bulk density (BD) and contents of soil organic C (SOC), sand and clay.

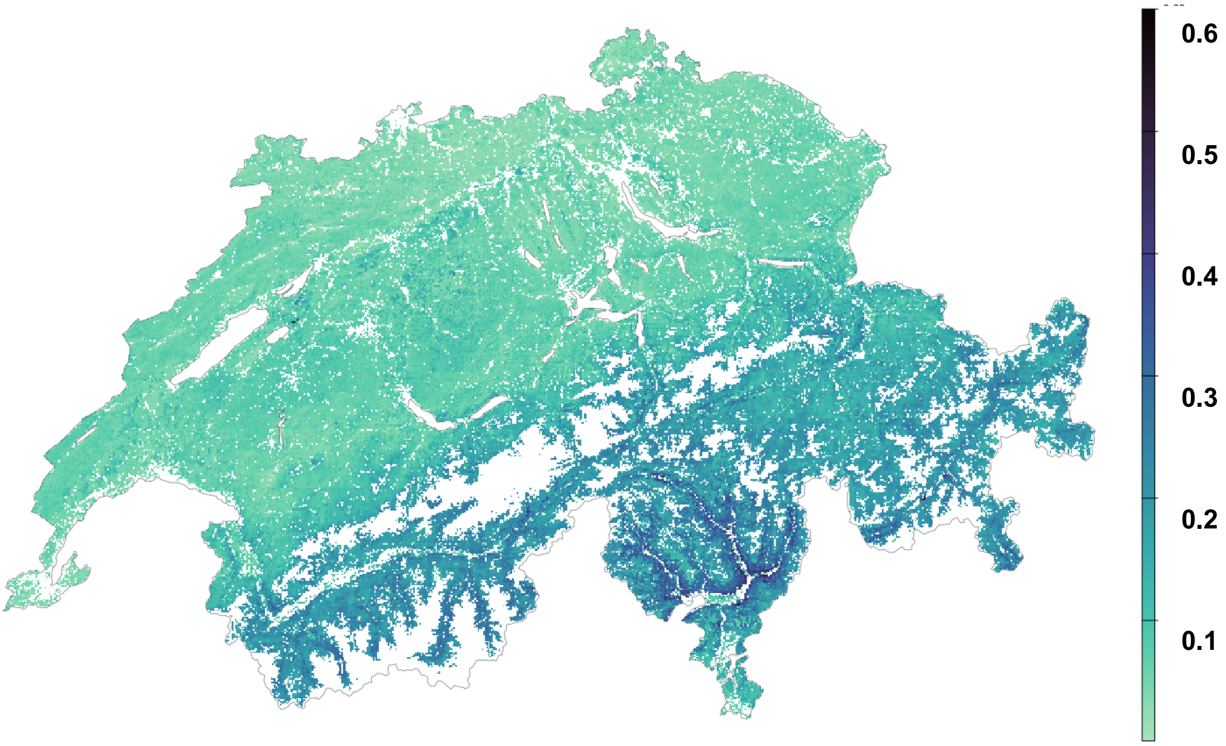

Figure 30: Map of soil saturated conductivity (K_{sat}), in cm s^{-1}, estimated using a pedotransfer function (PTF) described by Saxton and Rawls (2006); the dependent variables of the function are bulk density (BD), field capacity and wilting point described above and sand, clay and soil organic C (SOC) contents.

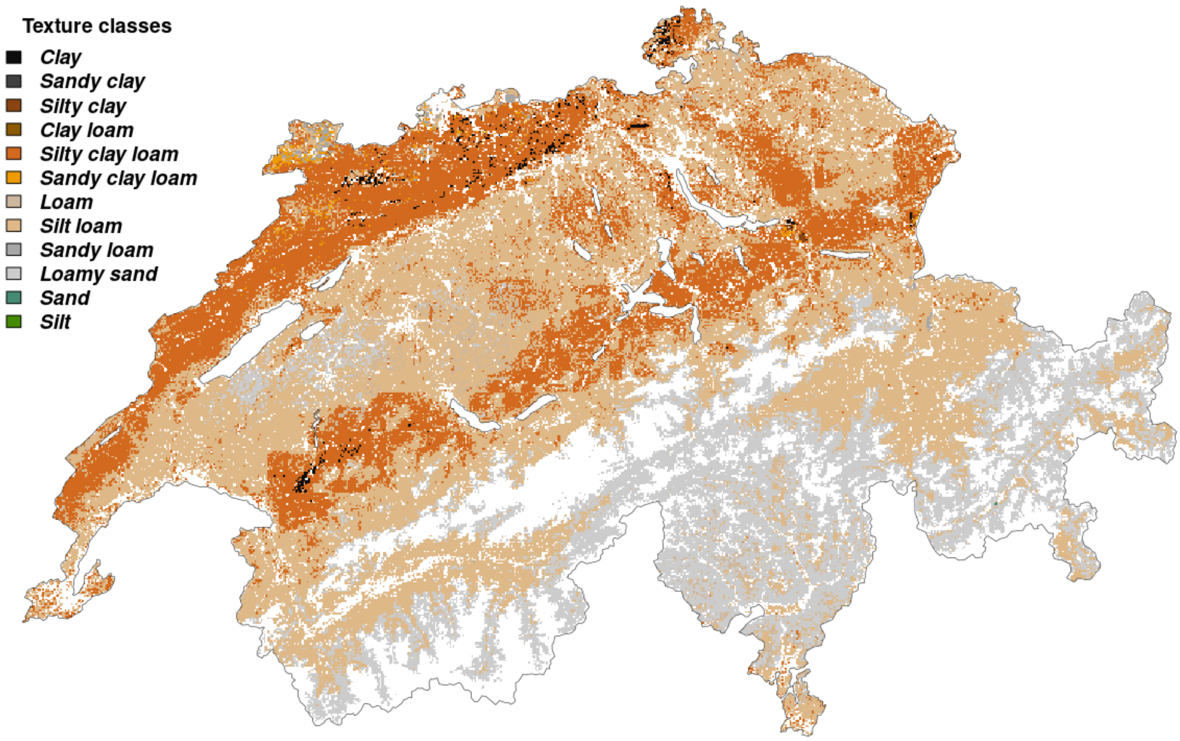

Figure 31: Map of soil texture classes produced from clay, silt and sand content maps.

10.5 Pedoclimatic combinations

The combination of 26 strata, 2 land use categories, 12 soil texture classes and 5 soil thickness classes formed the set of 3120 pedoclimatic combinations used for regional simulations. To avoid computational effort for model simulations of non-representative conditions, the pedoclimatic units were ordered descending by area and only those cumulatively adding up to 98% of the total area (grasslands + croplands) were selected for simulation. The pedoclimatic combinations not included in the simulation setup presented areas with less than 60 ha each. This procedure reduced the number of pedoclimatic combinations considered for simulation to less than 900 simulation units. In the final compilation of modeled values, mean values of N_2O emission for each land use category/subcategory were assigned to the pedoclimatic combinations not included in the simulation.

10.6 Management data

A standardized and oversimplified management scheme was applied for each land use category in this first regional simulation of N_2O emissions. For croplands, an 8-year crop rotation scheme was adopted based on information from long-term field experiments conducted in Switzerland and described in *Section 5.1.1*. Specifically, the main source used as a basis for defining the crop sequence and all the management practices adopted, including sowing (date), fertilization (date, type and amount), soil preparation (type and date) and harvesting (type and date) was the conventional treatment (*CONFYM2*) from the DOK experiment, after the year 2000. An adjustment was made to the rotation to include rapeseed in the crop rotation as this is an important crop type in Switzerland. To make this adjustment, the management practices associated with this crop were based on the Oensingen experiment (*Section 5.1.1*). Therefore, the basic crop rotation used for the simulation of croplands is shown in *Figure 32* below. The frequency of crops in this rotation is in line with the proportion of its cultivated areas in Switzerland, for example with a predominance of winter wheat (FAOSTAT, 2022). In the rotation, grass-clover leys covers about 2.4 of the 8 years, *i.e.*, approximately 30% of the rotational time, which is very consistent with the share of grass-clover leys in cropland areas (Wüst-Galley et al., 2019).

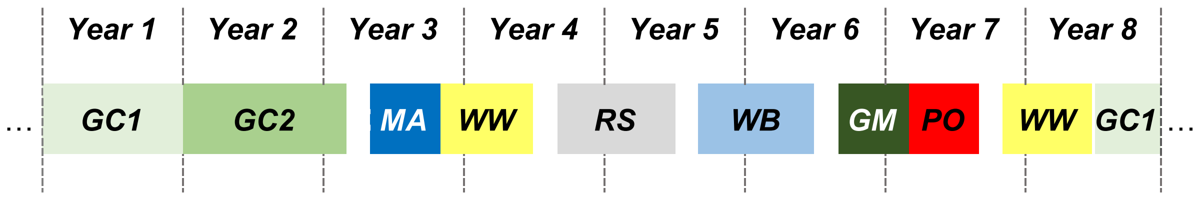

Figure 32: Eight-year crop rotation used as the basis for DayCent simulations. GC1: grass-clover ley (first year), GC2: grass-clover ley (second year), MA: grain or silage maize, WW: winter wheat, RS: rapeseed, WB: winter barley, GM: green manure, PO: potatoes.

To capture the effect of the interaction between crop growth and weather conditions over the years, respecting the proportion of the crops in the rotation, 8 different rotations were included in the simulations based on the above-mentioned scheme (*Figure 32*) with a sequential one-year shift. This means that management schedules[7] of eight different crop rotations were created as illustrated below, using theoretical crop types from A to H as example.

- *Rotation 1:* …**ABCDEFGH**...
- *Rotation 2:* …**BCDEFGHA**...
- *Rotation 3:* …**CDEFGHAB**...
- *Rotation i:* …
- *Rotation 8:* …**HABCDEFG**...

[7] these are input files used in the DayCent simulations; in these files the management is defined in detail, such as dates of sowing, plowing, harvest and type of fertilizer.

All the eight different management schedules were run for each pedoclimatic combination (see *Section 10.5 above*). The mean value of modeled soil N_2O emissions from the eight different management schedules was assigned to each pedoclimatic combination for further compilation of the final results.

As for croplands, some of the management assigned to grassland areas was based on field experiments conducted in Switzerland. One main field experiment used as a basis for defining the management was the one conducted in Oensingen (*Section 5.2.1* above). For grassland categories that were hardly represented in the field experiments (mainly the different pasture types), management schedules were created based on the 'Principles for the fertilization of agricultural crops in Switzerland' (GRUD) (Huguenin-Elie et al., 2017). Besides the information regarding N amounts, we considered the usual frequencies of mowing in meadows or grazing in pastures indicated in this guide, according to (i) the class of management intensity and (ii) the class of altitude, which were both associated with the agricultural zones defined above in *Section 10.1* above. In management schedules created based on the GRUD, the dates of practices (cuts or grazing) were defined considering a likely range of period of management according to the usual practices in a given category. For example, 6 to 7 grazing events per year were considered in intensive pastures in the valley region (agricultural zone A1), ranging from April to October, and only 2 to 3 grazing events were considered for extensive pastures in the mountain region (agricultural zone A3), concentrated in the period from June to August. To be consistent with the simulations for croplands, eight different schedules were created for each grassland subcategory by means of one-year shifts in the years of a basic 8-year management schedule created based on field experiments or information described in the GRUD.

10.7 Results of modeled N_2O emissions from Swiss agricultural soils

To illustrate results of the simulation of N_2O emissions for agricultural soils in Switzerland, we show in the *Figure 33* below the results of annual emissions for the year 2021. Even with the oversimplification of the management, this first regional simulation allows some first general inferences about N_2O emissions based on the process-based modeling approach used in the present project. In the Swiss Plateau, where cropland areas are concentrated, emissions are clearly higher compared to other regions dominated by grassland categories with lower degrees of management intensity. In addition to greater N inputs throughout the year, more frequent physical disturbance of the soil (*e.g.*, seedbed preparation), likely explains the higher emissions in the plateau. This is an important source of N_2O emissions that is well captured by DayCent in the field experiments (see results in the *Section 8.1* above). The plateau is also a region with trends towards higher values of soil density, associated with cultivation (*Figure 27*), and lower values of K_{sat} (*Figure 30*). The combination of higher BD, resulting in lower soil porosity, and lower K_{sat}, resulting in slower soil drainage, is a condition that favors N_2O emissions associated with low soil oxygenation (Bateman and Baggs, 2005; Zhu et al., 2013). It is also noted that the annual N_2O emissions, considering all pedoclimatic combinations and all the 32 years of simulations, varying from 0.54 to 4.78 kg N N_2O ha^{-1} yr^{-1}, reflects well the main range of values observed in the field experiments for croplands (*Figure 15*) and grasslands (*Figure 23*).

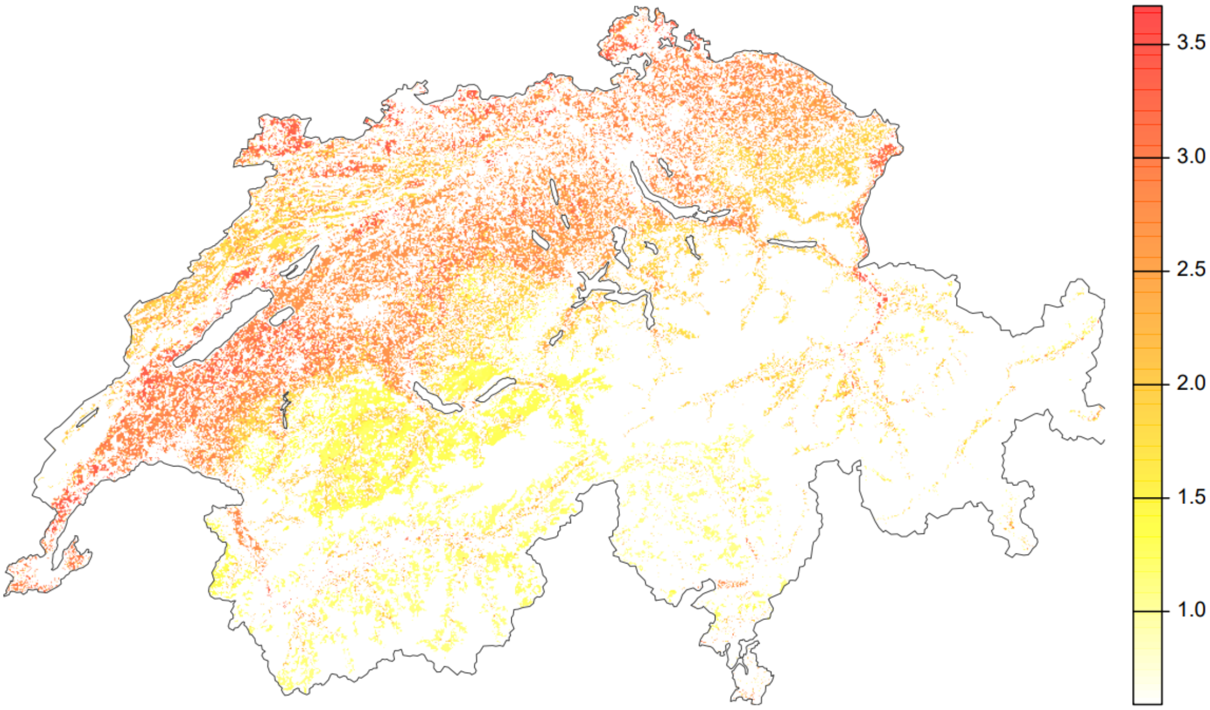

Figure 33: Map showing preliminary results for modeled N_2O emissions, in kg N ha^{-1}, from agricultural soils in Switzerland (year 2021). Strongly simplified management information was used for these simulations.

11 Conclusions and perspectives

In this project we focused on three critical steps towards setting up a model-based inventory for N_2O emissions from Swiss agricultural soils. Based on extensive field data, we were able to calibrate and evaluate the performance of the model DayCent and we gathered and processed necessary input data for first, simplified country-scale simulations of N_2O emissions.

Overall, based on comparisons against extensive field observations, the results of this project suggest that DayCent is an adequate model for reporting N_2O emissions from Swiss agricultural soils with complex management, diverse crop rotations on croplands and different levels of management intensity for grasslands. Our results showed that DayCent simulations were clearly more accurate than EF approaches. 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 plant residues on the inter-seasonal variability of background N_2O emissions, which has been recognized as a major contribution to total emissions. Other important factors, such as N and water use efficiency by plants are not accounted for by EF approaches. Considering these factors is key to reliably predict the impact of mitigation practices on soil N_2O emissions. Management alternatives towards emission abatement can only be tested by considering the major processes involved, which are simulated by ecosystem models such as DayCent.

Obtaining more precise management data is the next task towards establishing more accurate model-based estimates of N_2O emissions at a regional level. This challenge is also faced by other countries that apply models to report N_2O emissions from agricultural soils. For instance, the use of DayCent in the U.S. is coupled with a detailed systematic survey of land-use and management activity from all over the country conducted by the National Resources Inventory[8] and supplemented by several other sources of information[9], which serve as the basis for DayCent simulations of SOC stocks, CH_4 emissions from rice cultivation, and soil-based N_2O emissions for the inventory of national GHG emissions.

In Switzerland, new time series of precise land use geodata are available (“Landwirtschaftliche Kulturflächen”/ “Surfaces agricoles cultivées”) (FOAG, 2024). In combination with surveys of management activity at cantonal and national levels this information, could provide robust support for regional simulations of N_2O emissions. A very challenging step is how to extrapolate this information to past years (back to 1990). This will be a central point for the development of a model-based approach used for the national inventory.

[8] National Resources Inventory (NRI) is a statistically-based sample including ~500 thousand survey locations in the U.S., complemented with the Cropland Data Layer (CDL) from the National Agricultural Statistics Service (USDA-NASS). Please see more details in US-EPA (2023).

[9] Conservation Effects and Assessment Project (CEAP) collects more detailed cropland management activity data at a subset of NRI survey locations. Gradient boosting, a machine learning technique, is used to extrapolate management practices to all NRI locations. It includes data of tillage practices, mineral fertilization, manure amendments, cover crop management, and dates of sowing and harvest. Fertilizer types and rates by crop type for different regions of the U.S. are also provided by USDA Economic Research Service, Agricultural Resource Management Surveys (ARMS) and USDA-NASS. To determine the trends in tillage management, CEAP data are combined with Conservation Technology Information Center (CTIC) data and OpTIS remote-sensing data product. Please see more details in US-EPA (2023).

Acknowledgements

This study was funded by the Swiss Federal Office for the Environment (A. Schellenberger; "Prozessorientierte Modellierung der direkten N_2O-Emissionen landwirtschaftlicher Böden (LACHSIM)"; Contract Numbers 17.0083.PJ / S043-1410 and 17.0083. PJ / BAFU-D-598A3401/454). 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 ALLENVI ("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 N_2O 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 N_2O 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. Measuring infrastructure for the research conducted at Graswang and Fendt was provided by the TERENO Bavarian Alps/Pre-Alps Observatory, funded by the Helmholtz Association and the Federal Ministry of Education and Research (BMBF).

We would like to thank all the contributors who provided datasets and support for modeling and data processing, including:

- Melannie D. Hartman – Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, USA;
- Magdalena Necpalova and Johan Six – Sustainable Agroecosystems Group, ETH Zurich, Department of Environmental Systems Science, Institute of Agricultural Sciences, Switzerland;
- Regine Maier, Lukas Hörtnagl, Iris Feigenwinter, Markus Staudinger and Nina Buchmann – Grassland Sciences Group, ETH Zurich, Department of Environmental Systems Science, Institute of Agricultural Sciences, Switzerland;
- Maike Krauss, Colin Skinner and Paul Mäder – Research Institute of Organic Agriculture (FiBL), Department of Soil Sciences, Frick, Switzerland.
- Bernard Nicolardot – UMR Agroecology, AgroSup Dijon, French National Research Institute for Agriculture, Food and Environment (INRAE), Université Bourgogne Franche-Comté, Dijon, France;
- Christophe R. Flechard, Philippe Le Roy and Thierry Morvan – UMR Soils, Agricultural and Hydrological Systems, Spatialization (SAS), French National Research Institute for Agriculture, Food and Environment (INRAE), Agrocampus Ouest, Rennes, France;
- Carolin Boos, Benjamin Wolf and Ralf Kiese – Institute for Meteorology and Climate Research, Karlsruhe Institute of Technology, Garmisch-Partenkirchen, Germany;
- Felix Stumpf – Kompetenzzentrum Boden (KOBO), Bern, Switzerland;
- Beat Rihm – Meteotest, Bern, Switzerland;
- Reto Meier – Federal Office for the Environment (FOEN), Bern, Switzerland;
- Luca Nembrini, Robin Giger, Fabio Elvedi, Christof Ammann, Pierluigi Calanca and Chloé Wüst-Galley from Agroscope, Climate and Agriculture Group, Zurich, Switzerland.

Appendix I

Estimates of N_2O emissions from cropland sites using IPCC's emission factors

Estimation of N_2O emissions (kg N ha^{-1}) based on the emission factor (EF) approach follows the Intergovernmental Panel on Climate Change (IPCC) Guidelines (Hergoualc'h et al., 2019; Klein et al., 2007). The calculations in the present study were adapted to report emissions per crop cycle instead of annual values. We used following equations:

$$N_2O_{Agg} = (F_{sn} + F_{on} + F_{cr} + F_{som}) \times EF_1 \qquad \text{(Eq. A.1)}$$

$$N_2O_{Dis} = (F_{sn}) \times EF_{1sn} + (F_{on} + F_{cr} + F_{som}) \times EF_{1nsn} \qquad \text{(Eq. A.2)}$$

Where:

$N_2O\text{-}N_{Agg}$= total N_2O emissions estimated by aggregated emission factor, in kg N ha^{-1}.

$N_2O\text{-}N_{Dis}$= total N_2O emissions estimated by disaggregated emission factors, in kg N ha^{-1}.

F_{sn}= synthetic fertilizer N inputs, kg N ha^{-1}.

F_{on}= animal manure, compost, slurry and other organic N inputs, kg N ha^{-1}.

F_{cr}= N returned to soil as crop residue (aboveground and belowground), including N_2-fixing crops, kg N ha^{-1}.

F_{som}= N mineralized in soil associated to loss of SOC, kg N ha^{-1}.

EF_1= aggregated emission factor for N_2O emissions from N inputs, kg N_2O-N (kg N input)$^{-1}$. A default value of 0.01 was considered following the IPCC guidelines (Klein et al., 2007).

EF_{1sn}= disaggregated emission factor for N_2O emissions in wet climates from synthetic fertilizer N inputs, kg N_2O-N (kg N input)$^{-1}$. The value of 0.016 was used following the IPCC guidelines (Hergoualc'h et al., 2019).

EF_{1nsn}= emission factor for N_2O emissions in wet climates from N inputs other than synthetic fertilizer, kg N_2O-N (kg N input)$^{-1}$. The value of 0.006 was used following the IPCC guidelines (Hergoualc'h et al., 2019).

The estimates of F_{som} were based on field measurements of SOC stocks and a C:N ratio of 9.8, according to results obtained by Leifeld et al. (2007). If the amount of N in residues was not measured, F_{cr} was estimated based on default values of N content in above- and belowground residues, the ratio of aboveground residue to harvested yield and the ratio of belowground residue to harvested yield following the calculation procedures applied in the last Switzerland's Greenhouse Gas Inventory (FOEN, 2023). An annual value of 20 kg N ha^{-1} of N deposition was assumed as N input, based on estimates by Rihm and Achermann (2016) and Kosonen et al. (2019). The same EF values applied for synthetic N fertilizer were used to estimate N_2O emissions from N deposition.

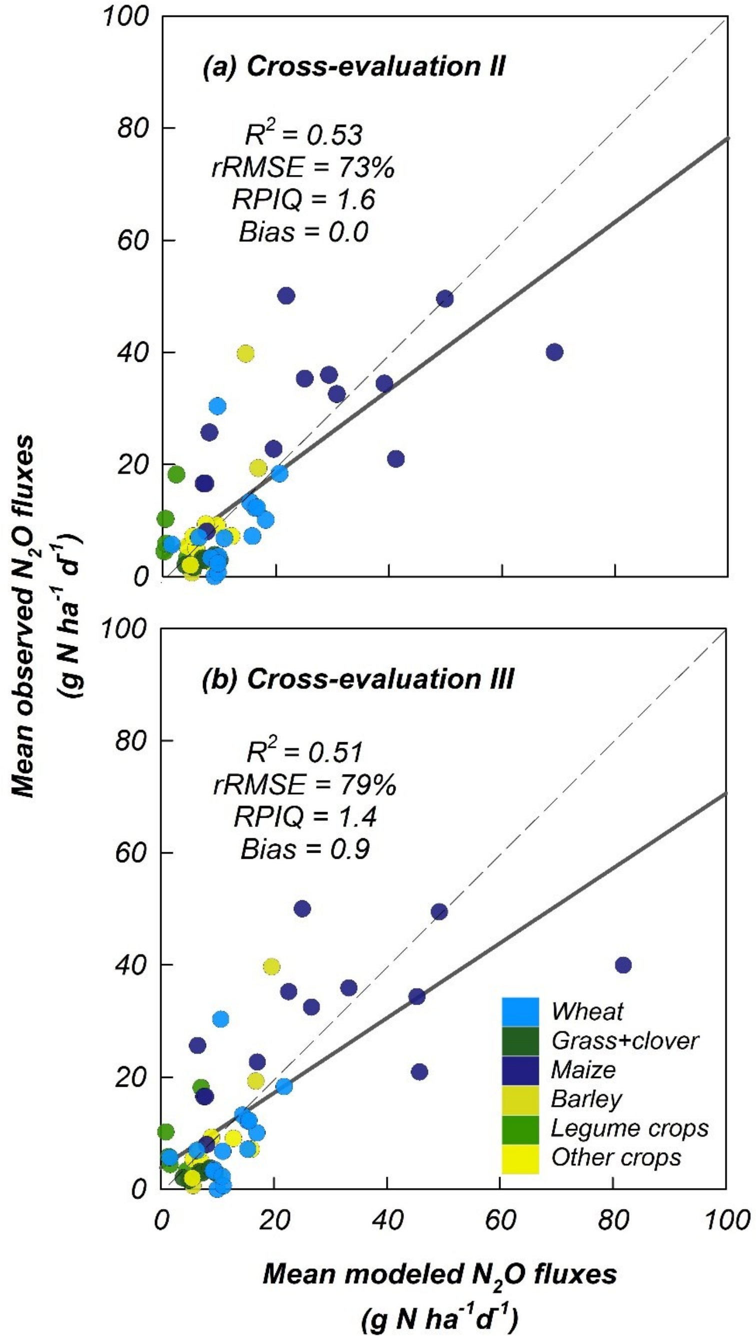

Figure A1: Mean modeled versus observed soil N_2O fluxes during different crop cycles of six sites in Switzerland and France. A leave-one-out (LOO) cross-evaluation was performed with (a) adjustment of only plant parameters, keeping management and N cycle parameters at their default values (b) adjustment of plant and management parameters, keeping N cycle parameters at their default values. The leave-one-out cross-evaluation was based on the use of the mean parameter value of all other sites except the one simulated. Each symbol stands for a crop cycle of a specific treatment and site.

Appendix II

Estimates of N_2O emissions N leaching from grassland sites using default factors of IPCC

Estimation of N_2O emissions (kg N ha^{-1}) based on the emission factor (EF) approach follows the Guidelines of Intergovernmental Panel on Climate Change (IPCC) (Hergoualc'h et al., 2019). The calculations of soil N_2O emissions from N inputs and deposited at grazing were based on the following equations:

$$N_2O_{direct}\text{-}N = N_2O\text{-}N_{N\ inputs} + N_2O\text{-}N_{prp}$$

where $N_2O_{direct}\text{-}N$ is the annual direct N_2O emissions, in kg N ha^{-1}; $N_2O\text{-}N_{N\ inputs}$ is the annual direct N_2O emissions derived from N all inputs, excluding excreta N deposited at grazing, in kg N ha^{-1}; and $N_2O\text{-}N_{prp}$ is the annual direct N_2O emissions derived from urine and dung deposited at grazing, in kg N ha^{-1}. The terms of the above-mentioned equation for estimating $N_2O_{direct}\text{-}N$ are detailed below:

$$N_2O\text{-}N_{inputs} = F_{sn} \times EF_{1sn} + (F_{on} + F_{cr} + F_{som}) \times EF_{1nsn}$$

$$N_2O\text{-}N_{prp} = F_{prp,cpp} \times EF_{3prp,cpp} + F_{prp,so} \times EF_{3prp,so}$$

where:

$N_2O_{direct}\text{-}N$= annual direct N_2O emissions, in kg N ha^{-1}.

$N_2O\text{-}N_{inputs}$ = annual direct N_2O emissions derived from N inputs, in kg N ha^{-1} (it does not include excreta N deposited at grazing).

$N_2O\text{-}N_{prp}$ = annual direct N_2O emissions derived from urine and dung deposited at grazing, in kg N ha^{-1}.

F_{sn}= synthetic fertilizer N inputs, kg N ha^{-1}.

F_{on}= animal manure, compost, slurry and other organic N inputs, kg N ha^{-1} (it does not include excreta N deposited at grazing).

F_{cr}= N returned to soil as plant residue (aboveground and belowground), including N_2-fixing plants, kg N ha^{-1}.

F_{som}= N mineralized in soil associated to loss of SOC, kg N ha^{-1}.

EF_{1sn}= disaggregated emission factor for N_2O emissions in wet climates from synthetic fertilizer N inputs, kg N_2O-N (kg N input)$^{-1}$. The value of 0.016 was used considering the disaggregated approach in the refinement of the IPCC guidelines (Hergoualc'h et al., 2019). It means that this value of 0.016 applies only for N inputs from synthetic fertilizer.

EF_{1nsn}= emission factor for N_2O emissions in wet climates from N inputs other than synthetic fertilizer, kg N_2O-N (kg N input)$^{-1}$. A value of 0.006 was used was used considering the disaggregated approach in the refinement of the IPCC guidelines (Hergoualc'h et al., 2019), that is, lower value than for synthetic fertilizers.

F_{prp}= amount of urine and dung deposited by grazing animals, kg N ha^{-1} (please see equation below). The acronym "*cpp*" refer to cattle, poultry and pigs and "*so*" refer to sheep and other animals.

EF_{3prp} = emission factor for N_2O emissions derived from excreta N deposited at grazing. The acronym "*cpp*" refer to cattle, poultry and pigs and "*so*" refer to sheep and other animals. The values are 0.004 for "*cpp*" and 0.003 for "so" (Hergoualc'h et al., 2019).

The calculation of F_{prp} was performed by using the following equation:

$$F_{prp} = \sum_T \left(N_T \times Nrate_T \times \frac{TAM_T}{1000} \times GP_T \right)$$

N_T= number of head of livestock of species per category *T*. Cattle and sheep were the only categories included in the present study (Fuchs et al., 2018; Merbold et al., 2021).

$Nrate_T$ = default N excretion rate, kg N (Mg animal mass)$^{-1}$ day^{-1}. The default values for Western Europe are 0.50 for cattle and 0.36 for sheep (Gavrilova et al., 2019).

TAM_T = typical animal mass for livestock category T, kg animal^{-1}. The default values for Western Europe are 600 for cattle and 40 for sheep (Gavrilova et al., 2019).

GP_T =grazing period with animals from the category T.

The N loss by leaching was calculated as follows:

$$N_{leaching} = (F_{N\ inputs} + F_{prp}) \times Frac_{leach}$$

where $N_{leaching}$ is the annual leached N (sum of organic and mineral forms), in kg ha^{-1}; $F_{N\ inputs}$ is the sum of N inputs, excluding excreta N deposited at grazing, in kg ha^{-1} and F_{prp} is the total amounts of N as urine and dung deposited at grazing, in kg ha^{-1}. The value F_{prp} was considered to be zero in the present study because there was no grazing in the sites with N leaching measurements (see *Section 5.2.1* of the report). $Frac_{leach}$ is the fraction of the N lost by leaching, defined as 0.24 kg leached N (kg N input)$^{-1}$ in the refinement version of the IPCC guidelines (Hergoualc'h et al., 2019). The terms of the above-mentioned equation for estimating $N_{leaching}$ are detailed below:

$$F_{N\ inputs} = F_{sn} + F_{on} + F_{prp} + F_{cr} + F_{som}$$

The F_{cr} value is only considered for grasslands with renewal (Hergoualc'h et al., 2019), which is not the case in our study. Besides of that, N inputs associated with F_{som} was assumed to be a negligible source of N_2O emission. According to the IPCC guidelines, this input is only considered in cases with net C losses indicating N mineralization (Hergoualc'h et al., 2019). Permanent grasslands under the pedoclimatic conditions in the region of the present study have presented a slight positive net change in C stocks, *i.e.* no net mineralization (FOEN, 2023). To keep a consistent comparison with the DayCent estimates and observed emissions, an annual value of 20 kg N ha^{-1} of N deposition was added to the N inputs, based on estimates by Rihm and Achermann (2016) and Kosonen et al. (2019). The same EF values applied for synthetic N fertilizer were used to estimate N_2O emissions from N deposition.

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