

What matters when? Temporal development of drivers and sources of nitrous oxide emissions in winter wheat

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Abstract. Agriculture is the largest anthropogenic source of nitrous oxide (N₂O), primarily due to nitrogen (N) fertilization. Understanding how the influence of key drivers and the relative contribution of source processes change throughout the cropping season is crucial for developing effective strategies to mitigate N₂O emissions. In this study, we combined high-resolution eddy covariance (EC) flux measurements, explainable machine learning (ML), and stable isotope analyses over one winter wheat cropping season and the subsequent summer cover crop season, at a temperate site in Switzerland. The SHAP-based driver analysis identified two phases, as particularly vulnerable to N₂O losses: crop establishment and early spring, were identified as critical periods for N₂O emissions. Both were characterized by a mismatch between N supply and plant demand, resulting in surplus soil mineral N and elevated N₂O fluxes under favorable environmental moisture and temperature conditions. Gross primary productivity (GPP), used as a proxy for crop activity and N uptake, suppressed demand, showed a consistent negative effect on N₂O emissions, especially under high soil moisture, highlighting fluxes supporting the importance of active vegetation in mitigating emissions as a competing N sink. Stable isotope source partitioning, based on stable isotopes, revealed identified denitrification as the dominant process of N₂O production, driven by pathway during the early-spring post-fertilization period, consistent with poor soil drainage and high soil moisture. Cumulative N₂O emissions over the nine-month winter wheat season, the Tier 1 N₂O emission factor was 1.8%, with cumulative emissions of reached 5.5 kg N₂O-N ha⁻¹, offsetting 70% of the net CO₂ uptake, with yield-scaled emissions of 1.1 kg N₂O-N Mg⁻¹ grain, both values exceeding those typically reported for wheat. Our findings emphasize the need to better synchronize N supply with crop demand and to adopt agronomic practices that promote rapid crop establishment to mitigate N₂O emissions highlight the value of combining EC, explainable ML, and stable isotope approaches to resolve the temporal dynamics of N₂O emissions and identify critical windows for targeted mitigation in cropping systems.

Keywords: arable land; nitrous oxide; winter wheat; cover crop; eddy covariance; stable isotopes; driver explainable machine learning

30 1 Introduction

Nitrogen (N) is an essential nutrient for crop production, and the use of N fertilizers plays a central role in ensuring global food security (Erisman et al., 2008; Liang, 2022). However, a large part of the applied N is lost to the environment due to misalignment between the application (amount and timing) and crop demand (Ladha et al., 2005). Globally, only about 47% of total fertilizer N input is taken up by crops, with the remainder lost primarily through nitrate (NO_3^-) leaching and ammonia (NH_3) volatilization, contributing to water and air pollution (Lassaletta et al., 2014). Approximately 1% of the applied N (IPCC, 2019) is emitted as nitrous oxide (N_2O), a potent greenhouse gas (GHG) with a 100-year global warming potential (GWP_{100}) of 273 times that of CO_2 (Forster et al., 2021), and the dominant ozone-depleting substance of the current century (Portmann et al., 2012; Ravishankara et al., 2009). Together with carbon dioxide (CO_2) and methane (CH_4), N_2O represents one of the three major greenhouse gases contributing to anthropogenic climate forcing, with agricultural soils being a significant source of all three (Nabuurs et al., 2022). Despite accounting for a relatively minor fraction of N losses, the climate impact of N_2O makes its mitigation a key priority in sustainable agricultural management. Direct N_2O emissions from agricultural N additions ~~representare~~ the largest source of anthropogenic N_2O emissions, ~~contributingaccounting for~~ 56% of global emissions over the past decade (Tian et al., 2024), with more than half (55%) originating from soils following fertilizer application. The remaining fraction is attributed to manure excreted on pastures and manure management (Epper et al., 2025; Tian et al., 2024). In Switzerland, N_2O emissions account for approximately 30% of total agricultural GHG emissions (FOEN, 2025~~6~~). At both EU and Swiss levels, policies have been introduced to reduce N losses from agriculture and mitigate associated environmental impacts, such as the EU Nitrates Directive (European Commission, 1991) and Switzerland's Water Protection Ordinance (Swiss Federal Council, 1998). However, despite the well-documented climate effects of N_2O , binding measures specifically targeting N_2O mitigation are still lacking (Epper et al., 2025). This regulatory gap hinders the development and implementation of effective mitigation strategies, leaving a major source of agricultural greenhouse gas emissions largely unaddressed.

N_2O in soils is primarily produced through microbial nitrification and denitrification, ~~processes that are regulated by a complex interplay of dynamic~~ (Butterbach-Bahl et al., 2013). Several interacting factors, including ~~the~~ N substrate availability ~~of N substrates~~ (i.e., NH_4^+ and NO_3^-), soil moisture, temperature, pH, and ~~availability of~~ labile carbon ~~(Butterbach-Bahl et al., 2013; supply, affect both production of N_2O and reduction of N_2O to N_2 , the final product of denitrification~~ (Davidson, 1991; Rummel et al., 2025; Saggiar et al., 2013; Smith, 2017). Agronomic operations such as fertilization and tillage increase N availability and stimulate microbial N_2O production (Chatskikh and Olesen, 2007; Shcherbak et al., 2014). Recent studies also highlight the role of actively growing vegetation as a dynamic N sink that competes with microbes for N substrates, thereby reducing their availability for N_2O production and mitigating N_2O emissions (~~Abalos et al., 2018~~; Feigenwinter et al., 2023; Maier et al., 2022; Timilsina et al., 2024). Accordingly, the N surplus, defined as the difference between total N inputs and outputs, correlates positively with N_2O emissions (Tallec et al., 2022; Van Groenigen et al., 2010). However, the spatio-temporal heterogeneity of environmental and management-related

drivers, along with the high temporal variability of N₂O fluxes, pose major challenges for identifying key drivers of N₂O ~~losses~~emissions throughout the cropping season. ~~Each phase~~Across the cropping cycle, from field preparation to post-harvest, ~~is controlled~~N₂O emissions are shaped by ~~distinct processes~~changes in soil environmental conditions, N availability, and their interactionsmanagement (Smith et al., 1998; Garnier et al., 2024). While many studies have explored the general relationships between individual drivers and N₂O emissions, to our knowledge, no study has systematically investigated how the relative importance of these drivers changes over the course of a cropping season. Therefore, our understanding of these temporal dynamics is still scarce, limiting the development of mitigation strategies because these may only be effective when aligned with the dominant emission controls at specific stages of the cropping season.

In addition to N₂O, croplands exchange substantial amounts of CO₂ and CH₄ with the atmosphere, which together determine their net greenhouse gas (GHG) budget (Carlson et al., 2017; Ciais et al., 2010; Schulze et al., 2009). CO₂ fluxes reflect the difference between photosynthetic carbon uptake and ecosystem respiration, whereas CH₄ fluxes from agricultural soils result from concurrent microbial production (i.e., methanogenesis) and oxidation (i.e., methanotrophy) (Le Mer and Roger, 2001). Quantifying these fluxes alongside N₂O is crucial for an integrated assessment of the cropland GHG budget and its response to environmental and management drivers.

To improve our understanding of the temporal dynamics of N₂O emissions and their contribution to the ~~full~~net GHG budget, continuous and spatially integrated measurements of N₂O fluxes are essential. Micrometeorological techniques such as eddy covariance (EC) enable continuous, high-frequency observations of N₂O fluxes, spatially integrating over entire fields (Feigenwinter et al., 2023; Lognoul et al., 2019; Maier et al., 2022, 2025). When EC-based N₂O flux measurements are combined with concurrent observations of key environmental and management-related drivers, they can provide valuable insights into the temporal dynamics of N₂O emissions and their controls throughout the cropping season. Building on high-resolution data provided by EC systems, machine learning (ML) algorithms offer powerful tools to model N₂O emissions (Gnisia et al., 2025; Goodrich et al., 2021; Hamrani et al., 2020). These ML models can capture non-linear relationships and complex interactions among environmental and management-related drivers and often outperform traditional statistical approaches in predictive accuracy (Philibert et al., 2013; Saha et al., 2021). Furthermore, model explanation techniques such as SHapley Additive exPlanations (SHAP; Lundberg and Lee, 2017) enhance the interpretability of ML models by quantifying the contribution of individual drivers, offering insights into the temporal evolution of driver importance (Krebs et al., 2025; Scapucci et al., 2024, 2025).

While ML models can identify which environmental and management variables most influence N₂O fluxes, they do not reveal the underlying microbial production processes. ~~This distinction~~Recent work has shown that modelling distinct N₂O emission regimes may help infer dominant production pathways (Lussich et al., 2026), but such attribution remains indirect. Nevertheless, such attribution is important because nitrification and denitrification respond differently to environmental conditions (Butterbach-Bahl et al., 2013; Davidson, 1991) and management (Buchen et al., 2018). Distinguishing between these two sources of N₂O is essential for developing targeted mitigation strategies and improving the accuracy of process-based biogeochemical models (Del Grosso et al., 2020). Stable isotope analysis, particularly of the intramolecular

distribution of ^{15}N (i.e., the so-called site preference, SP), offers a robust approach to identify the relative contributions of nitrification and denitrification to N_2O production (Toyoda and Yoshida, 1999). These ~~microbial~~ processes generate N_2O with distinct isotopic signatures due to differences in enzymatic mechanisms and substrate pools. Because SP is largely independent of the isotopic composition of precursor substrates, it enables robust source partitioning under field conditions (Decock and Six, 2013). Combined with ~~N~~nitrogen and ~~O~~oxygen stable isotope ratios ($\delta^{15}\text{N}$ and $\delta^{18}\text{O}$, respectively), SP ~~allows tracing~~can be used to trace the temporal development of N_2O -producing processes and constrain the extent of N_2O reduction to N_2 (Verhoeven et al., 2019; Yu et al., 2020).

The present study integrates continuous EC measurements, ML-based driver analysis, and stable isotope techniques to provide a comprehensive assessment of N_2O emissions over a winter wheat cropping season and the following short summer cover crop at a study site with ~~a~~-temperate climate in Europe. Specifically, we aimed to (i) quantify N_2O , CO_2 , and CH_4 fluxes and resulting GHG budgets throughout a winter wheat cropping season and the subsequent cover crop season, (ii) determine the temporal development of environmental and management driver contributions to N_2O fluxes, and (iii) identify the contributions of different microbial N_2O -producing processes and their temporal development after/during the weeks following a fertilization event.

2 Material and methods

2.1 Study site

The study site is a cropland field in Oensingen, canton of Solothurn, Switzerland. The site has a mean annual temperature of 10.1°C and receives an average of 1151 mm of precipitation per year (2004-2023). CO_2 and water vapor (H_2O) fluxes have been continuously measured at the site by ~~aan~~ EC station (CH-Oe2, part of FLUXNET; $47^\circ10'41.5''\text{ N}$, $7^\circ39'54.4''\text{ E}$; 465 m a.s.l.) since December 2003 (Emmel et al., 2018). The field where the station is positioned has an area of 1.55 ha, and the soil is ~~an~~classified as Eutric-Stagnic Cambisol with a silty clay ~~soil~~-texture. In the top 0.25 cm depth, the soil consists of 43% clay, 47% silt, and 10% sand, with 2.8% organic matter (Alaoui and Goetz, 2008). In the top 0.1 m depth, soil pH is 6.4 (Maier et al., 2025), and bulk density is 1.27 g cm^{-3} . Carbon and nitrogen stocks in the 0-0.7 m soil profile, derived from Emmel et al. (2018), are 18.6 kg C m^{-2} and 1.9 kg N m^{-2} , respectively. The field is managed according to an integrated farming label (IP ~~Swuisse~~), and follows the Proof of Ecological Performance (PEP; Swiss Federal Council, 2025). PEP sets baseline requirements for receiving direct payments, including rules for crop rotation, farm-based fertilizer use, and measures to protect soil and biodiversity. Over the past 20 years, the crop rotation included various annual crops, with winter wheat as primary crop. A temporary grassland (grass-clover mixture; STEFFEN 3003M, Samen STEFFEN AG) was established in 2020 and managed until its final cut in late September 2022, followed by herbicide application (Glyphosate) and direct-seeding of winter wheat. This study was conducted over one year, from September 2022 to October 2023, covering the last month of the temporary grassland, the full winter wheat growing season, and the subsequent cover crop season, a mixture of legumes, grasses, and forbs (Terra-FIT Quattro, Samen STEFFEN AG). Winter wheat (Montalbano,

130 bred by Agroscope and DSP) was sown on October 6, 2022, and harvested on July 15, 2023, with 5.03 t ha⁻¹ grain yield (dry matter). The winter wheat received three applications of mineral and organic (dairy slurry) fertilizers between late tillering and early stem elongation, summing up to 138 kg N ha⁻¹ (Table 1). After the harvest, the straw was removed from the field, and the soil was cultivated for the subsequent sowing of the summer cover crop. The cover crop was mulched in late September 2023, before the soil was cultivated again to prepare for the sowing of winter barley in early October 2023.

135 **Table 1. Main management activities conducted during the 2022-2023 measurement period at the cropland in Oensingen. Positive values for nitrogen (N) in/output (kg ha⁻¹) indicate inputs to the field, whereas negative values represent N exports. For organic fertilization the slurry application, total N is reported, with the which included 18 kg NH₄⁺-N fraction shown in parentheses ha⁻¹. Due to a sampling issue in 2023, slurry composition was estimated based on laboratory analysis of a 2024 sample from the same farm. Harvest-related N exports are reported as mean ± 1 standard deviation. Details on commercial products and additional management practices are provided in Table A1.**

Crop	Management activity	Date	N in/output (kg ha ⁻¹)
Grass-clover	Harvest	20 September 2022	- 40
	Herbicide application	3 October 2022	
Winter wheat	Sowing (direct seeding)	6 October 2022	+5.2
	Ammonium nitrate application	27 February 2023	+68
	Slurry application (40 m ³ ha ⁻¹ ; dairy)	28 February 2023	+43 total N
	Ammonium nitrate application	6 April 2023	+27
	Harvest (grain and straw)	15 July 2023	-113
Bare soil	Shallow tillage (cultivator; 0.05-0.1 m depth)	17 July 2023	
Cover crop	Sowing	27 July 2023	+1.4
	Mulching	25 September 2023	
Bare soil	Shallow tillage (cultivator; 0.05-0.1 m depth)	27 September 2023	

2.2 Eddy covariance flux measurements

2.2.1 Setup

145 The EC setup, situated at the center of the field, consisted of an ultrasonic anemometer (R3-50, Gill Instruments Ltd., Lymington, UK) that measured wind speed, and a laser spectrometer that measured N₂O and CH₄ concentrations at 10 Hz (GLA351-N2OM1, Los Gatos Research, Mountain View, CA, USA), as well as an enclosed infrared gas analyzer (IRGA) that measured CO₂ and H₂O concentrations at 20 Hz (LI-7200, LI-COR Biosciences, Lincoln NE, USA). The laser spectrometer was connected to an external pump (EV-A06, Ebara Technologies, Sacramento, CA, USA) and both were placed in temperature-controlled boxes. A 7 m long, 7.5 mm diameter unheated polyethylene/aluminum composite tube 150 (EATON Synflex 1300, Dublin, Ireland) was used to draw air to the laser spectrometer. The measurement height of the sonic anemometer was 2.17 m above ground, and the inlets of the laser spectrometer and the IRGA were mounted approximately

0.2 m below the sonic anemometer. While CO₂ and H₂O fluxes have been measured continuously since 2003, N₂O and CH₄ flux measurements were conducted during selected periods between 2018 and 2021 (Maier et al., 2025), followed by continuous measurements from 30 August 2022 to 5 October 2023 in the present study.

155 2.2.2 Flux processing

Half-hourly fluxes of CO₂, H₂O (i.e., as latent heat flux (LE)), as well as N₂O and CH₄ fluxes were calculated using the EddyPro software (version 7.0.9, LI-COR Environmental, Lincoln NE, USA) following established EC flux community protocols (Aubinet et al., 2012; Nemitz et al., 2018; Pastorello et al., 2020; Sabbatini et al., 2018). Raw high-frequency data underwent de-spiking and screening, in line with Vickers and Mahrt (1997), and wind components were aligned using a 2D rotation method (Wilczak et al., 2001). The time lag between the vertical wind component and scalar concentration of N₂O and CH₄ was set to a constant value, corresponding to the most frequently occurring lag (1.40 s for N₂O and 1.50 s for CH₄) identified through covariance maximization within a broad window (0-5 s) over the entire measurement period. In contrast, time lags for CO₂ and LE were determined dynamically through covariance maximization within narrow windows, based on prior lag distributions identified using a broader window. When no clear covariance peak was detected within the defined window, a default lag was applied (1.30 s for CO₂, 1.45 s for H₂O), corresponding to the most frequently identified lag in the earlier analysis. Spectral corrections addressed high-pass (Moncrieff et al., 2005) and low-pass filtering effects (Fratini et al., 2012). A correction for instrument separation was applied (Horst and Lenschow, 2009). The flux footprint model by Kljun et al. (2015) estimated the upwind area contributing to the measured flux.

2.2.3 Quality assessment and de-spiking

170 Data quality was assessed using a composite flag (QC0 = best quality, QC1 = medium quality, QC2 = bad quality), calculated with the Python library *diive* (v0.86.0; Hörtnagl, 2025). The flag included tests for (1) steady-state and integral turbulence characteristics (Mauder and Foken, 2004), (2) spectral correction factor (values with spectral correction factor > 4 were excluded), (3) IRGA signal strength, (4) completeness of the averaging interval (if <97% coverage within 30 min, value was excluded; Sabbatini et al., 2018), and (5) occurrence of spikes and drop-outs in the raw data after the statistical tests by Vickers and Mahrt (1997). Fluxes with the quality flag 2 (QC2) were excluded from further analyses. Storage terms (single point measurement) were added to all measured gas fluxes (Aubinet et al., 2001). CO₂ fluxes are referred to as net ecosystem exchange of CO₂ (NEE) from this point onwards. Absolute limits were applied to remove half-hourly fluxes outside plausible ranges, determined by analyzing typical ranges for highest-quality fluxes (NEE: - 60 to 50 μmol m⁻² s⁻¹; LE: -50 to 800 W m⁻²; N₂O: -3 to 30 nmol m⁻² s⁻¹; CH₄: - 30 to 80 nmol m⁻² s⁻¹). Outliers were further removed ~~using two~~ statistically by sequentially applying one or more of the following filters: a, as needed: rolling standard deviation, Hampel-filter applied separately for daytime, and nighttime periods, and a rolling z-score method, as these methods capture different types of anomalies. Finally, a friction velocity (u_{*}) filter (Papale et al., 2006) was applied to NEE, N₂O, and CH₄ fluxes to exclude periods with insufficient turbulence conditions. The threshold was determined using CO₂ fluxes, and a constant u_{*} threshold

of 0.092 m s^{-1} was used for the entire study period. After applying all quality checks, de-spiking, and u_* filtering, data coverage for fluxes over the entire measurement period was 50.8% for NEE, 68.5% for LE, 52.9% for N_2O fluxes, and 33.6% for CH_4 fluxes. Gaps were predominantly short (median: two records for NEE and CH_4 , one record for N_2O), with >99.6% lasting <1 day. Only one gap for NEE and five gaps for N_2O and CH_4 exceeded three days, and only one gap for N_2O and CH_4 exceeded seven days (none for NEE); maximum gap lengths were ~five days for NEE and ~nine days for N_2O and CH_4 (Table A2). Only the highest quality N_2O fluxes (QC0, 34.5% data coverage) were used for the driver analysis.

Further details on data quality control procedures and outlier removal methods are available in the project repository (Turco, 2025a). Flux rates are reported as $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ for NEE, $\text{nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$ for N_2O flux, and $\text{nmol CH}_4 \text{ m}^{-2} \text{ s}^{-1}$ for CH_4 flux, while cumulative fluxes are reported as g C m^{-2} (NEE, CH_4) or $\text{kg N}_2\text{O-N ha}^{-1}$ (N_2O).

2.2.4 Gap-filling and NEE partitioning

Gap-filling of N_2O and CH_4 fluxes was performed using ~~the~~ Random Forest (RF) ~~algorithm~~ regressor (Breiman, 2001) as implemented via the *diive* Python library (v. 0.86.0), based on the *scikit-learn* ~~(v1.15)~~ framework. Although a systematic comparison of gap-filling methods for eddy covariance N_2O fluxes is still lacking, RF has been shown to outperform conventional approaches for CH_4 fluxes (Irvin et al., 2021; Kim et al., 2020), supporting its use here for both non- CO_2 gases.

Predictor (i.e., driver) variables were selected based on their demonstrated predictive performance in previous studies (Feigenwinter et al., 2023; ~~Maier et al., 2022~~), including environmental data (and their lagged variants), management information (expressed as time since event), and timestamp features. Environmental variables comprised soil temperature, precipitation (in absolute terms and time since occurrence), and soil water content. For model training and evaluation, each dataset was randomly split into training and test subsets, with 25% of the data reserved for testing. Model performance differed markedly between gases. For N_2O fluxes, the model achieved an R^2 of 0.79, with a MAE of $0.40 \text{ nmol m}^{-2} \text{ s}^{-1}$ and a RMSE $\text{nmol m}^{-2} \text{ s}^{-1}$ of 0.90. In contrast, performance for CH_4 fluxes was poor, with an R^2 of -0.05, a MAE of $5.8 \text{ nmol m}^{-2} \text{ s}^{-1}$, and a RMSE of $8.7 \text{ nmol m}^{-2} \text{ s}^{-1}$. Although we did not systematically assess gap-filling uncertainty as a function of gap length (Bigaignon et al., 2020; Taki et al., 2018), this limitation is partly mitigated by the generally short gap lengths in our dataset (Table A2).

For NEE and LE, gap-filling was conducted using the Marginal Distribution Sampling (MDS) method (Reichstein et al., 2005), implemented in R via the *REddyProc* package (v. 1.3.2; Wutzler et al., 2018). Input variables for MDS included global radiation, air temperature, and vapor pressure deficit. NEE was subsequently partitioned into gross primary production (GPP) and ecosystem respiration (R_{eco}) using the night-time method (Reichstein et al., 2005), also implemented in *REddyProc* (Wutzler et al., 2018). Additional methodological details and code are available in the project repository (Turco, 2025a).

2.3 ~~Calculating N₂O emission factor~~Calculation of net GHG exchange and GHG budgets

215 ~~The N₂O emission factor (EF) for winter wheat was calculated by dividing the cumulative N₂O-N emissions attributable to fertilization (excluding background fluxes) by the total amount of N from synthetic and organic fertilizers. This calculation excluded background fluxes and followed the IPCC Tier 1 approach (IPCC, 2019). The background N₂O flux was calculated as the average of gap filled fluxes, omitting 30 day post fertilization periods to remove the short term fertilization effects. The resulting EF is expressed as the percentage of the applied N that is emitted as N₂O-N.~~

220 ~~The net GHG budgets for CO₂~~budget

Cumulative N₂O, and CH₄, and CO₂ fluxes were calculated separately for the winter wheat ~~and cropping season and the subsequent cover crop period using gap-filled flux datasets. The winter wheat cropping seasons (282 and 60 days, respectively), covering season was defined as~~ the period from sowing to harvest, ~~using gap filled flux datasets (see Sect. 2.2.4 for gap filling procedure).~~ while the cover crop period was defined as the period from cover crop sowing to mulching. To express fluxes in terms of CO₂-equivalents, global warming potential (GWP₁₀₀) values of 273 for N₂O and 27 for CH₄ were applied, in accordance with current estimates (Forster et al., 2021). The sum of N₂O, CH₄ and CO₂, i.e., the cumulative fluxes expressed in CO₂-equivalents (CO₂-eq), is hereafter referred to as net GHG exchange (NGHGE). This term is used to distinguish the EC-based atmospheric exchange from the net GHG budget, which additionally accounts for lateral C imports and exports.

230 The net GHG budget was derived from the C budget, which combines NEE with lateral C fluxes from management (imports and exports). C exports comprised harvested grain and straw, and C imports comprised organic fertilizer additions. Exports were treated as positive fluxes (C removal from the ecosystem) and imports as negative fluxes (C addition). The C budget was converted to CO₂-eq using the molecular mass ratio of CO₂ to C, then N₂O and CH₄ fluxes (in g CO₂-eq) were added to obtain the net GHG budget, following Ammann et al. (2020). Negative values indicate a net GHG sink, positive values a net GHG source.

235 To assess the sensitivity of NGHGE to friction velocity (u_*) filtering (Table A3), cumulative N₂O, CH₄ and CO₂ fluxes and the resulting NGHGE were calculated under alternative u_* thresholds, corresponding to the 16th and 84th percentiles of the bootstrapped u_* threshold distribution (CUT16 and CUT84, respectively), in addition to the default threshold (CUT50; median), following Pastorello et al. (2020).

240 The N₂O emission factor (EF) for the winter wheat season was calculated by dividing the cumulative N₂O-N emissions from sowing to harvest by the total amount of N from mineral and organic fertilizers. The resulting EF is expressed as the percentage of the applied N that is emitted as N₂O-N. Because no unfertilized control treatment was available, non-fertilization-induced emissions could not be subtracted. The resulting value, therefore, represents an apparent EF rather than an IPCC Tier 1 EF. To account for N₂O emissions beyond the winter wheat season, we additionally calculated an annual apparent EF for the one-year period starting at winter wheat sowing, including the bare-soil period after harvest and the

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subsequent cover crop period. This metric was calculated as cumulative annual N₂O-N emissions divided by the fertilizer N applied during the same period.

2.4 Meteorological and soil variables

The meteorological variables air temperature and relative humidity (CS215, Campbell Scientific Ltd., Logan UT, USA), atmospheric pressure (PAA-33X, Keller AG, Switzerland), short- and longwave radiation (CNR4, Kipp & Zonen, Delft, Netherlands), photosynthetic photon flux density PPFD (BF5, Delta-T Devices, United Kingdom), and precipitation (heated tipping bucket rain gauge, Lambrecht meteo GmbH, Germany) were measured continuously at the EC station. Soil water content and soil temperature were also measured continuously close to the EC station along one soil profile (at 0.05, 0.15, 0.3, and 0.5 m soil depths) using 5TM sensors (Decagon Devices, Inc., Pullman WA, USA). All meteorological measurements were recorded at one-minute time resolution and, after screening for outliers, averaged to 30-minute values (precipitation was summed). Water-filled pore space (WFPS; Eq. 1) was calculated for each soil depth as:

$$WFPS = \frac{SWC}{1 - \frac{BD}{PD}} * 100 \quad (1)$$

where SWC is the volumetric soil water content (in m³ m⁻³), BD is the bulk density (in g cm⁻³), with values of 1.16, 1.40, and 1.33 g cm⁻³ for the 0-0.05, 0.15-0.3, and 0.3-0.5 m depth intervals, respectively, obtained from Emmel et al. (2018), and PD is the particle density, assumed to be 2.65 g cm⁻³ (Danielson and Sutherland 1986). Because SWC was measured at a single soil profile, absolute WFPS estimates may not fully represent spatial variability across the EC footprint. However, similar SWC dynamics observed at an independent sensor profile located a few meters away indicated that temporal patterns were representative. The WFPS conversion further relied on bulk density values from Emmel et al. (2018), which may not fully reflect topsoil conditions during this experiment. Therefore, uncertainty is expected mainly in absolute WFPS values rather than in temporal WFPS dynamics.

2.5 Soil chamber measurements and stable isotope analyses

Five opaque static PVC (polyvinyl chloride) chambers, each with a volume of 17.7 L and a surface area of 0.07 m², were deployed at five randomly selected locations within a 12 m radius of the EC station (Fig. 1). The chambers were first deployed on 24 February 2023, before the first fertilization event, and positioned to enclose plants from two adjacent wheat rows. To ensure that regular field management could continue unhindered, the chambers were removed immediately after sampling when management operations were scheduled before the next sampling date and subsequently reinstalled at the same positions for the following measurements. In total, six sampling campaigns were conducted between 24 February and 17 March 2023, encompassing the period around the first fertilizations (27 and 28 February) and two campaigns later in the season (31 May and 19 July). The sampling was performed around midday (typically between 11:00 and 13:00 local time) to minimize diurnal variability in fluxes. For each chamber and time point, two headspace samples were collected: one immediately after chamber closure (t₀), and one after a 1-hour enclosure period (t₆₀). Air samples were drawn from the

chamber headspace with a 60-mL syringe. For subsequent N₂O concentration analysis, 20 mL of the air sample was injected into pre-evacuated 12 mL vials. For stable isotope analyses, 180 mL of the air sample was injected into pre-evacuated 110 mL serum crimp vials. During each sampling campaign, a soil sample was collected for each chamber by combining two soil
 280 cores (0-0.1 m depth) taken approximately 0.3 m from the chamber edge. The pooled samples were placed into Schott tubes, which were immediately sealed with Parafilm, enclosed in plastic bags, and stored in a cooling box before being transferred to a freezer at -18 °C. Soil water was later extracted from the samples using cryogenic vacuum distillation (Ehleringer and Osmond, 2000). The stable oxygen isotope ratio ($\delta^{18}\text{O}$) of the extracted water was then measured using an isotope ratio mass spectrometer (IRMS; DeltaplusXP, Finnigan MAT, Bremen, Germany) and expressed in the delta notation referenced to the
 285 Vienna Standard Mean Ocean Water (V-SMOW) in ‰ (Eq. 2) as:

$$\delta^{18}\text{O} = \frac{R_{\text{sample}}}{R_{\text{reference}}} - 1 \quad (2)$$

where R denotes the ratio of $^{18}\text{O}/^{16}\text{O}$.

N₂O gas samples were analyzed for their stable N and oxygen isotope ratios ($\delta^{15}\text{N}^{\text{bulk}}$, $\delta^{18}\text{O}$, respectively) ~~and~~ as well as the site preference (SP-N₂O) using a trace gas preparation unit (Elementar, Manchester, UK) coupled to an IsoPrime100 IRMS
 290 (Elementar, Manchester, UK). Calibration and data correction followed the procedure described in Verhoeven et al. (2019) and in Gallarotti et al. (2021), including the use of multiple working standards and correction for instrumental drift, span, and linearity. In addition, instrument performance was regularly assessed using standards treated as samples (Werner and Brand, 2001), ensuring data quality and interlaboratory comparability (Mohn et al., 2014). Site preference (SP) represents the difference between the N isotope ratios at the central (α) and terminal (β) N positions of the N₂O molecule. Unlike
 295 $\delta^{15}\text{N}^{\text{bulk}}$, SP-N₂O is independent of the initial substrate, making it a more direct indicator of the N₂O production pathway (Toyoda et al., 2002). The isotopic signature of emitted N₂O was calculated using the following two-point mixing equation (Eq. 3):

$$\delta^z X = \frac{[\text{N}_2\text{O}]_e \cdot \delta^z X_e - [\text{N}_2\text{O}]_s \cdot \delta^z X_s}{[\text{N}_2\text{O}]_e - [\text{N}_2\text{O}]_s} \quad (3)$$

where $[\text{N}_2\text{O}]_s$ and $[\text{N}_2\text{O}]_e$ are the N₂O mixing ratios [ppb] at t_0 and t_{60} , respectively, measured using a gas chromatograph
 300 equipped with an electron capture detector (456-GC, Scion Instruments, Livingston, WLO, UK), while $\delta^z X_s$ and $\delta^z X_e$ are the corresponding isotope ratios (‰). A threshold of 30 ppb in N₂O concentration increase ($\Delta[\text{N}_2\text{O}] = [\text{N}_2\text{O}]_e - [\text{N}_2\text{O}]_s$) was used to exclude flux estimates for which the change in N₂O concentration during the chamber closure was too small to yield reliable isotopic signatures (Harris et al., 2020b). N₂O fluxes on four of the eight sampling dates, March 1, 3, 6, and 17, exceeded this threshold and were subsequently included in the analyses. Thus, isotope-based process identification was
 305 restricted to the three weeks following the first fertilization events at the end of February 2023 (Table A1).

To determine the main production pathways of N₂O, a dual isotope mapping approach was used, relating i) $\delta^{18}\text{O}$ -N₂O to SP-N₂O, and ii) $\delta^{15}\text{N}^{\text{bulk}}$ -N₂O to SP-N₂O. The mixing endmembers for nitrification (Ni), heterotrophic bacterial denitrification (bD), nitrifier denitrification (nD), and fungal denitrification (fD) were chosen according to Yu et al. (2020). The $\delta^{18}\text{O}$ -N₂O endmembers of bD, nD, and fD were adjusted by the mean $\delta^{18}\text{O}$ of soil water to account for the oxygen isotopic signature of

310 the substrate (Lewicka-Szczebak et al., 2020). Since no measurements of the $\delta^{15}\text{N}$ of soil N precursors were available, a $\delta^{15}\text{N}$ value of 0‰ was assumed for precursor nitrate and ammonium in the $\delta^{15}\text{N}^{\text{bulk}}\text{-N}_2\text{O}$ vs. $\text{SP-N}_2\text{O}$ map. The contributions of different $\text{N}_2\text{O-N}_2\text{O}$ production pathways and the residual fraction of unreduced N_2O (r) were estimated with the FRAME software, implementing a Markov Chain Monte Carlo model (Lewicki et al., 2022). The FRAME model was configured using process-specific mean values and fractionation factors from Yu et al. (2020), and the $\delta^{18}\text{O-N}_2\text{O}$ mean values were
315 corrected for $\delta^{18}\text{O-H}_2\text{O}$. FRAME was run using the mixing-reduction scenario, in which N_2O from different production pathways is mixed before partial reduction to N_2 . The reduced N_2O fraction is reported as $(1 - r)$, where r represents the residual fraction of N_2O remaining after reduction. To test sensitivity to the assumed order of mixing and reduction, the alternative reduction-mixing scenario was also tested, in which denitrification-derived N_2O is reduced before mixing with N_2O from the other pathways.

320 2.6 Vegetation and soil measurements

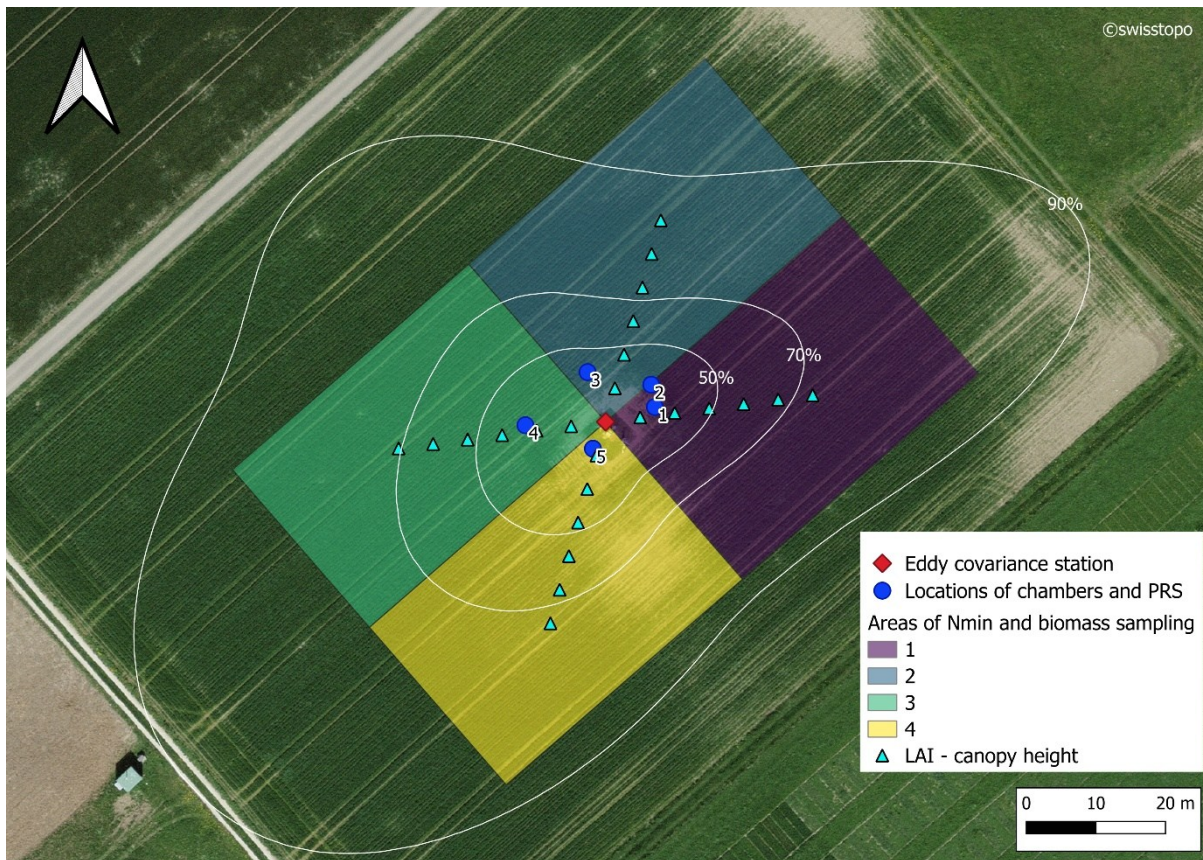
Leaf area index (LAI), vegetation height, and phenological development stages were monitored throughout the study. From March to July 2023, measurements were conducted at 2- to 3-week intervals to capture the growth dynamics during the most active vegetative period of winter wheat, and at key developmental stages before and after this period. LAI and canopy height were measured at six locations spread 5 m apart along four transects originating from the EC station (Fig. 1). LAI was
325 measured using a LAI-2000 Plant Canopy Analyzer (LI-COR Biosciences, USA) by taking one above-canopy and six below-canopy readings for each transect. Under clear sky conditions, measurements were conducted towards the North to avoid direct sunlight on the lens. Vegetation height was determined by measuring the height of an expanded polystyrene plate of 0.25 m² dropped on top of the vegetation at each spot (Ammann et al., 2007). Phenological development stages of winter wheat were identified according to the BBCH-scale (Meier, 2018) for five plants randomly selected in the field.

330 Aboveground biomass (AGB) was sampled monthly, using a harvest frame with a defined area of 0.1 m². Three samples were randomly collected at each of the four defined field sections (Fig. 1), and entire wheat plants were cut 2 cm above the ground. At harvest, grain and straw were sampled separately to estimate C and N exports from the field. The dry weight was determined after drying all plant samples at 60 °C for 48 hours. The dried samples were further processed by first cutting the biomass into smaller pieces, then a subsample was ground to a fine powder with a ball mill (MM200, Retsch, Germany).
335 Finally, about 4 mg was weighed into small tin capsules, and carbon (C) and N concentrations (in %) were determined with a Flash EA 1112 elemental analyzer (Thermo Italy, former CE Instruments, Rhodano, Italy).

Soil mineral N was measured during the wheat cropping season, to quantify the instantaneous extractable inorganic N pools. Soil samples were collected five times using a machine-assisted soil core sampler. ~~The soil samples were collected~~ within the same field sections used for AGB sampling, with ten to fifteen soil cores taken at each section and bulked for each soil
340 depth (0-0.3, 0.3-0.6, and 0.6-0.9 m). Ammonium (NH_4^+) and nitrate (NO_3^-) were extracted by an external laboratory using a 0.01 M CaCl_2 solution at a 1:4 soil-to-solution ratio, following the Swiss reference method (Buerge, 2020) established by the Federal Agriculture Research Center, Agroscope. Concentrations were photometrically determined by the same laboratory

and reported in mg N per 100 g of dry soil. Soil mineral N ($N_{\min}$) was then calculated in kg N ha⁻¹ using the same reference method.

345 Plant Root Simulator probes (PRSTM, Western Ag, Saskatoon, Canada) were used as a complementary measure of plant-
available N supply over time. In contrast to $N_{\min}$ measurements, which provide a snapshot of extractable inorganic N at the
time of sampling, PRS probes integrate ion supply to exchange membranes over the burial period and therefore provide a
time-integrated estimate of available N supply. Measurements of plant-available soil N complemented soil sampling from
March to September 2023. Three ~~Plant Root Simulator~~PRS sets ~~(17.5 cm² surface area each; PRSTM, Western Ag,~~
350 ~~Saskatoon, Canada),~~ each consisting of one anion and one cation exchange resin probe, ~~(17.5 cm² surface area each),~~ were
buried at 0-0.1 m soil depth. This depth was chosen to target the soil layer most strongly affected by management and where
root density and nutrient uptake are highest. The probes were positioned along the wheat inter-row at the same five locations
used for chamber measurements (Fig. 1). The probes were replaced every two to three weeks, resulting in seven burial
periods. No probes were buried in June due to technical issues, nor in the second half of July due to tillage and sowing
355 operations. Prior to shipment to Western Ag for analyses, the PRS probes were rinsed with deionized water and stored at
5°C. Extraction of NH₄⁺ and NO₃⁻ with 0.5 mol L⁻¹ HCl was conducted by pooling all three PRS sets from each location,
yielding one value per location and sampling period (in µg N per ~~17.5~~10 cm² per time of burial). Since all NH₄⁺
measurements were below the detection limit (except for one sample), we excluded NH₄⁺-N from further analyses.



360 Figure 1. Experimental setup at the study site in Oensingen during the 2022-2023 measurement period. The red diamond marks the eddy covariance station; white lines delineate the 50%, 70%, and 90% average footprint areas (based on the Kljun et al., 2015 model); blue dots indicate locations of manual chambers and plant root simulator (PRS) probes; colored rectangles show areas for Nmin and aboveground biomass sampling; triangles denote fixed locations for LAI and canopy height measurements. Orthophoto: Federal Office of Topography swisstopo.

365 2.7 Investigating the temporal development of N₂O drivers

2.7.1 XGBoost model

To investigate biotic and abiotic drivers of N₂O fluxes, we implemented a regression model based on eXtreme Gradient Boosting (XGBoost; Chen & Guestrin, 2016), using the *xgboost* library in Python. The dataset was aggregated into 4-hour intervals to balance temporal resolution with noise reduction. Only highest-quality measured N₂O fluxes (QC0) were used for the driver analysis. An initial set of predictors included variables previously identified as key drivers of N₂O fluxes (Butterbach-Bahl et al., 2013; Feigenwinter et al., 2023; Goodrich et al., 2021; Maier et al., 2022, 2025), namely soil temperature, WFPS (at depths of 0.05, 0.15, and 0.3 m), precipitation, time since key management events (soil preparation, fertilization, and harvest), and gross primary productivity (GPP). GPP was selected as the indicator of vegetation performance instead of leaf area index (LAI) and canopy height because of its higher temporal resolution and its strong

375 correlation with aboveground crop N content observed during the winter wheat season (Fig. A1). To represent ~~N-availability~~
~~from recent~~ fertilization ~~inputs~~, we ~~included~~ ~~used~~ the cumulative ~~fertilizer~~ N applied over the preceding 30 days (~~total N~~; kg N
~~ha⁻¹~~), ~~a~~). This window ~~length that reflects~~ ~~was chosen to capture~~ the ~~typical duration of enhanced soil N-availability and N₂O~~
~~emissions following fertilizer short-term post-application period commonly considered in event-based reporting, not~~
~~accounting for longer-lived or legacy fertilization effects~~ (Bouwman, 1996; Cowan et al., 2020; Qian et al., 2025). In
380 addition, we derived lagged values, rolling means (sums for precipitation and GPP), and first-order time derivatives (i.e.,
rates of change) for environmental variables, calculated over 12-, 24-, and 48-hour intervals. ~~Soil mineral N was not included~~
~~as a predictor because it was measured only on discrete dates and, given the highly dynamic nature of soil N availability,~~
~~could not be meaningfully interpolated to subdaily (4-hour) resolution. Fertilization-related variables and GPP were~~
~~therefore used as proxies for recent N input and crop activity, respectively, with GPP interpreted as an indicator of plant N~~
385 ~~demand rather than an independent driver separated from soil N availability.~~

Recursive feature elimination (Guyon et al., 2002) was applied to systematically identify the most informative predictors
from the initial variable set. The cumulative N applied over the preceding 30 days emerged as the strongest important
predictor of N₂O fluxes, followed by time since ~~fertilization, time since~~ soil preparation, ~~time since fertilization,~~ and the 48-h
~~(preceding) rolling mean of lagged~~ WFPS at 0.3 m depth. To minimize multicollinearity while retaining the key biotic and
390 abiotic drivers, we selected the variable with the highest ranking from each category of predictors. The final set of predictors
included: cumulative N applied over the past 30 days, time since fertilization, time since soil preparation, the 48-h
~~(preceding) rolling mean of lagged~~ WFPS at 0.3 m depth, the change in WFPS at 0.3 m depth over the preceding ~~48~~24 h, the
48-h (preceding) rolling mean of soil temperature at 0.3 m depth, and the cumulative GPP over the preceding 48 h. For
WFPS, both its ~~lagged~~ absolute value and short-term temporal change were retained, as they capture distinct dimensions of
395 soil moisture dynamics. Similarly, both cumulative ~~N~~ applied ~~N~~ and time since fertilization were included, reflecting their
complementary roles in describing N availability and timing of fertilization events.

~~Following variable selection, model-~~ The dataset was split chronologically: the first 80% was used for feature selection and
~~hyperparameter optimization, and the final 20% was reserved as an independent hold-out set.~~ Hyperparameters were
optimized ~~using~~ ~~10~~ within this training period using a randomized search with 5-fold cross-validation. ~~To account for~~
400 ~~temporal autocorrelation and avoid overfitting, while also providing representative coverage of the measurement period, we~~
~~employed a custom time block strategy. This approach involved an 80/20 split between training and validation, with the~~
~~validation set comprising randomly selected, non-overlapping time blocks that together represented 20% of the available~~
~~data. This splitting strategy was consistently applied throughout the modeling workflow, including during cross-validation~~
~~and final model evaluation. (Table A5).~~ Model performance was ~~then~~ evaluated ~~using~~ ~~on the independent hold-out period,~~
405 ~~based on~~ root mean squared error (RMSE), ~~which quantified the average deviation between predicted and observed values,~~
~~and mean absolute error (MAE), and~~ the coefficient of determination (R²), ~~calculated both during cross-validation and for the~~
~~final model.~~

The final XGBoost model used the following hyperparameter values: `colsample_bytree = 1`, `gamma = 0`, `learning_rate = 0.05`, `max_depth = 10`, `min_child_weight = 2`, `n_estimators = 100`, and `subsample = 0.65`, and was trained with early stopping (10 rounds) to prevent overfitting. Cross-validation results showed a R^2 of 0.60 and a RMSE of $1.1 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$ on the validation set, while the training set showed a R^2 of 0.98 and a RMSE of $0.29 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$. The final model, trained with early stopping (10 rounds) to prevent overfitting, optimized model achieved a R^2 of 0.70 and a RMSE of 1.14 $R^2 = 0.36$, RMSE = $1.19 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$, and MAE = $0.71 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$ on the independent hold-out set (training performance: $R^2 = 0.76$, RMSE = $1.04 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$ on the test set⁻¹, and MAE = $0.47 \text{ nmol N}_2\text{O m}^{-2} \text{ s}^{-1}$). Although the model tended to overestimate low fluxes and underestimate peak fluxes, it reproduced the temporal dynamics of N_2O fluxes (Fig. A2).

2.7.2 SHAP analyses

To interpret model outputs and investigate the temporal dynamics of predictor (i.e., driver) contributions to N_2O fluxes, we applied SHAP (SHapley Additive exPlanations; Lundberg and Lee, 2017), a model-agnostic interpretability framework based on cooperative game theory. SHAP was implemented using the SHAP Python library in combination with the XGBoost model trained for N_2O flux prediction. Specifically, we used TreeExplainer (Lundberg et al., 2020), a SHAP implementation optimized for tree-based models such as XGBoost. This method with the XGBoost model, which decomposes each model prediction into additive contributions from individual predictors, quantifying how much each ~~onedriver~~ increases or decreases the prediction relative to a defined baseline.

Because the SHAP analysis, the aimed to interpret temporal patterns within the observed dataset rather than to forecast future N_2O fluxes, the model used for SHAP interpretation was trained on the full dataset (including the hold-out period). This allowed driver contributions to be estimated across the complete measurement period. The SHAP baseline is was defined by as the expected model prediction over a reference dataset that represents typical input representing non-management-dominated conditions and serves as a reference state for calculating feature contributions (Lundberg et al., 2020; Molnar, 2025). To construct this reference dataset, we excluded the 30 days following fertilization or and soil preparation to best represent average, undisturbed environmental conditions. This ensured that SHAP values reflected the influence of the predictor variables in relation to typical conditions, without being skewed by the absence of recent management events. SHAP values were used to quantify the absolute contribution of each predictor to the model output. For interpretability, SHAP values were then normalized by dividing each SHAP value by the sum of all their absolute SHAP values for that each prediction. This transformation yielded to yield relative, unitless relative contributions that are independent of prediction magnitude and whose absolute values sum to one across all predictors at each time step, while preserving the effect direction of each predictor's effect. This enabled and enabling a time-resolved assessment of the relative importance of individual predictors. contribution of all drivers.

For interpretation of the SHAP analyses interpretability, we grouped related variables by summing their aggregated SHAP values across related predictors to assess quantify the overall net contribution of broad driver categories. Specifically, SHAP

values ~~for the~~ cumulative N applied and time since fertilization were ~~combined to represent the contribution of fertilization related drivers, labeled as summed to define the~~ ‘N fertilization’. Likewise, SHAP values for ~~driver~~, whereas WFPS and its temporal derivative were ~~aggregated to capture the influence of soil moisture dynamics, referred to as~~ ‘summed to define the’ ‘WFPS’ ~~driver~~. For clarity, we refer to ‘time since soil preparation’ as ‘soil disturbance’. ~~From this point onward, we will refer to predictor variables as ‘drivers’ in the manuscript.~~, ‘48-h (preceding) rolling mean of soil temperature at 0.3 m depth’ as ‘soil T’, and ‘cumulative GPP over the preceding 48 h’ as ‘GPP’. Hereafter, we use the term ‘drivers’ to denote predictors.

All statistical analyses were conducted in Python (version 3.9.13) using NumPy (Harris et al., 2020a), pandas (McKinney, 2010), SciPy (Virtanen et al., 2020), ~~and~~ scikit-learn (Pedregosa et al., 2011), ~~and~~ shap (Lundberg and Lee, 2017). Data visualization was performed with Matplotlib (Hunter, 2007) and Seaborn (Waskom, 2021). The Python scripts used for these analyses and visualizations are available on GitHub and archived on Zenodo (Turco, 2025b6).

3. Results

3.1 Environmental conditions and vegetation growth

~~The cropping season for~~ Winter wheat ~~at Oensingen started was sown~~ on 6 October 2022, following ~~the final cut of a~~ temporary ~~grassland (grass-clover), which was cut ley~~ on 20 September 2022 (Table 1). ~~Large precipitation events followed this final cut, totaling 103 mm in 15 days (Fig. 2a), resulting in increased WFPS values (Fig. 2b). During this~~ The period, ~~topsoil temperature (0.05 m depth) ranged between 12 and 15 °C (Fig. 2c). Throughout after the final cut was wet, with 103 mm of precipitation in 15 days, which increased WFPS (Fig. 2a,b). During~~ the winter wheat ~~growing~~ season, cumulative precipitation amounted to 698 mm. ~~However, with~~ rainfall ~~was unevenly distributed, with concentrated in~~ November to ~~December 2022 (33%) and March to April 2023 accounting for 33% and (29% of the total precipitation, respectively (Fig. 2a).%)~~. A dry ~~spell period~~ occurred ~~between from~~ late December 2022 ~~and to~~ early March 2023, but, although topsoil WFPS ~~in the topsoil~~ remained above 60% (Fig. 2b). ~~In contrast,), while~~ a second ~~drought dry~~ period ~~between from~~ mid-May ~~and to~~ late June 2023 ~~coincided with warmer conditions and led to a decline in reduced~~ WFPS throughout the soil profile (20 to 20-30% in the ~~top upper~~ 0.3 m) ~~of the soil~~. Topsoil temperature ranged ~~between from~~ 0.4 ~~and to~~ 24.6 °C and showed a typical ~~temporal course~~ °C, with ~~lowest minimum~~ values ~~from December 2022 to February 2023 in winter~~ and ~~highest maximum~~ values in July 2023. ~~The~~ Winter wheat development of LAI ~~was slow~~ during the ~~growing season followed the seasonal weather pattern, remaining low throughout winter and early spring before increasing steadily, with LAI remaining low until March (Fig. 2d). LAI increased rapidly~~ from late March 2023 (Fig. 2d). Canopy development ~~and~~ peaked ~~in late at the end of~~ May, shortly before anthesis (i.e., flowering; Table A2) in early June 2023. During June’s dry and warm conditions, canopy desiccation and signs of water stress became apparent, accompanied by the onset of senescence as seen in the decline of LAI. ~~Crop management started with A4). The first two fertilization events early in the season (fertilizer applications were conducted on 27- and 28 February 2023) during late tillering (Table A2), approximately one week before the onset of rainfall~~

that ended the winter dry spell. The last fertilization event was conducted, and the final application was on 6 April during the early stem elongation phase (6 April), following a period of increased temperature. After the harvest of winter wheat in mid July 2023 (Table 1), the soil was cultivated and a cover crop was sown at the end of July, accompanied by intense rainfall and declining soil temperature. The. During the short summer cover crop season was short and characterized by increasing soil moisture, particularly in the deeper soil layers (0.3–0.5 m; Fig. 2b), and by gradually period following wheat harvest and soil tillage, soil temperature remained variable before decreasing soil temperature (Fig. 2e). The season ended with mulching and soil cultivation attoward the end of September (Table 1), after which the soil was left bare until the sowing of the next crop on 4 October 2023. the period, while soil moisture increased, particularly in deeper soil layers (Fig. 2b,c), and cover crop development remained limited (Fig. 2d).

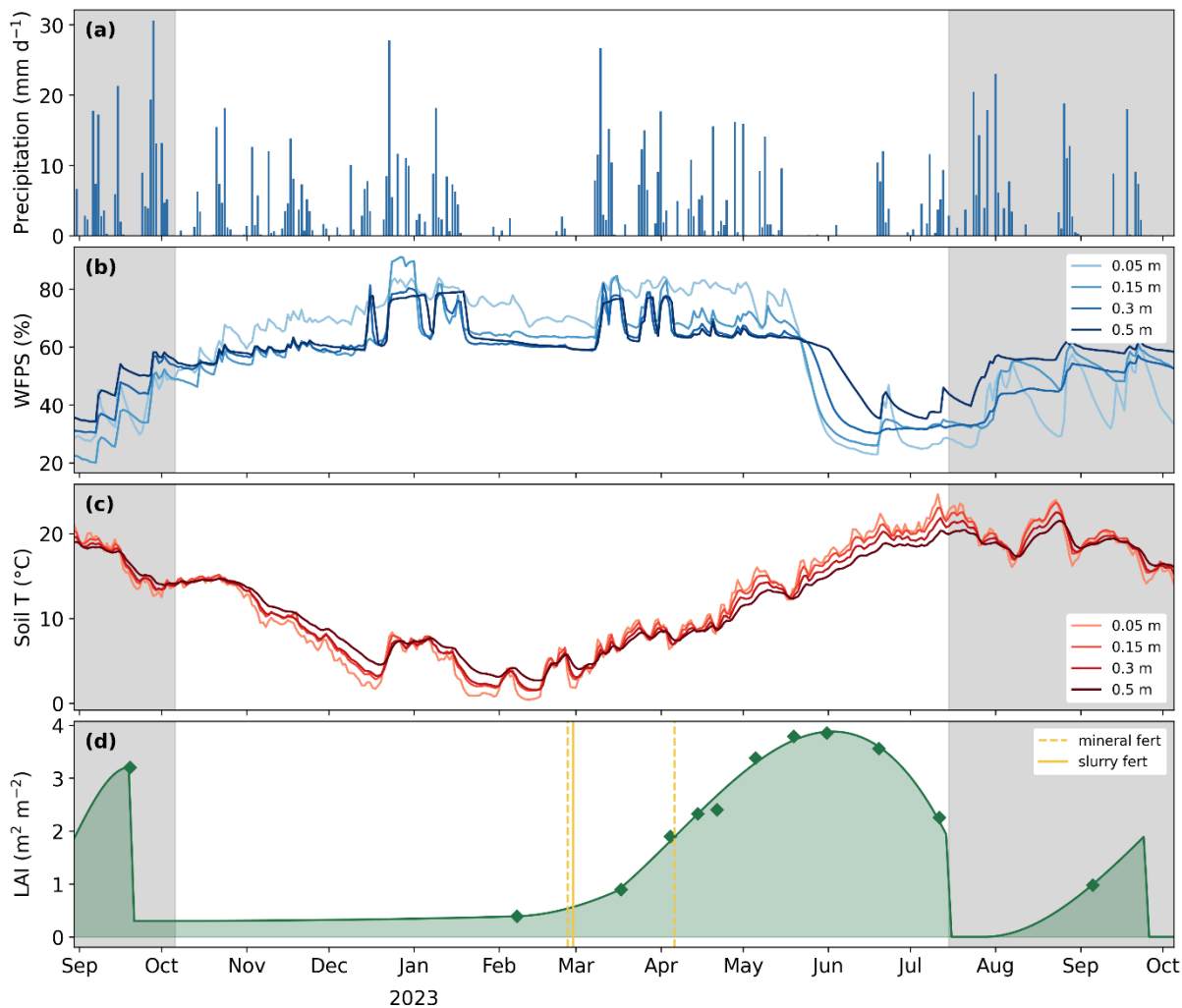


Figure 2. Environmental conditions and vegetation dynamics at the Oensing cropland from September 2022 to October 2023. The unshaded area corresponds to the winter wheat cropping season, while the shaded areas indicate the final phase of the preceding temporary grassland and the cover crop following the winter wheat harvest. (a) Daily precipitation sums; (b) daily

average water-filled pore space (WFPS) at 0.05, 0.15, 0.3, and 0.5 m soil depths; (c) daily average soil temperature (soil T) at the same depths as WFPS; (d) leaf area index (LAI), with diamonds indicating measured values and the line representing modelled values obtained using cubic splines. Yellow lines indicate fertilization (fert) events.

3.2 Greenhouse gas fluxes

3.2.1 Net ecosystem CO₂ exchange (NEE)

During the final regrowth phase of the temporary grassland in ~~October~~September 2022, daily mean NEE fluctuated around zero (-2.2 to +3.9 $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$; Fig. 3a). After the final grassland cut, NEE became positive, indicating a net release of CO₂. ~~Two weeks later, an~~Herbicide application ~~followed by and~~ direct seeding of winter wheat in early October 2022 further increased NEE, which reached a daily mean of +6.1 $\mu\text{mol m}^{-2} \text{ s}^{-1}$. In late October 2022, NEE gradually declined in response to decreasing soil temperature (Fig. 2c) and remained low but positive during the winter months (December ~~2022 to~~ February 2023), reflecting a small net release of CO₂. From early ~~to late~~March 2023, ~~daily mean onward~~, NEE decreased ~~from +2.3 to -3.5 $\mu\text{mol m}^{-2} \text{ s}^{-1}$ and became negative~~, indicating the onset of net CO₂ uptake. During peak crop growth in early May, daily mean NEE reached -10.5 $\mu\text{mol m}^{-2} \text{ s}^{-1}$, and the most negative half-hourly flux (QC0) was -48.2 $\mu\text{mol m}^{-2} \text{ s}^{-1}$. ~~With the onset of crop~~Following anthesis ~~at the end of May (Table A2)~~ and the ~~occurrence~~onset of dry soil conditions ~~(at the end of May~~ (Fig. 2b), NEE steadily increased, consistent with ~~reduced~~declining photosynthetic ~~CO₂ uptake, typical of this phenological phase in winter~~activity during wheat maturation. A small CO₂ emission peak, with daily mean NEE reaching up to +3.7 $\mu\text{mol m}^{-2} \text{ s}^{-1}$, occurred in late June, following rewetting after an extended dry period. From July to late August 2023, daily mean NEE remained positive (+1.9 to +7.7 $\mu\text{mol m}^{-2} \text{ s}^{-1}$), indicating net CO₂ release during late wheat maturation ~~as well as~~, after harvest and ~~subsequent early~~cover crop establishment. In late August ~~2023~~, NEE ~~was~~became negative ~~again~~, reflecting net CO₂ uptake due to the successful establishment of the cover crop. ~~Directly, before returning positive~~ after mulching ~~of the cover crop~~ and soil cultivation/tillage in late September, ~~the field became a net CO₂ source again (positive NEE)~~.

3.2.2 ~~Net ecosystem~~ N₂O fluxes

~~Net~~ N₂O fluxes showed pronounced temporal variations, with ~~very~~ low fluxes during winter 2022/2023 and highest emissions during crop establishment and after fertilization events. During the final grassland regrowth phase, daily mean N₂O fluxes were negligible (-0.3 to +0.6 $\text{nmol m}^{-2} \text{ s}^{-1}$; Fig. 3a), but increased markedly after winter wheat seeding, reaching ~~a~~ ~~daily mean of~~ +5.7 $\text{nmol m}^{-2} \text{ s}^{-1}$ on 22 October 2022 (Fig. 3b). This peak occurred after rainfall increased topsoil ~~(0.05 m)~~ WFPS from 51 to 62% (Fig. 2b), ~~while~~soil temperature ~~exceeded~~remained above 14 °C (Fig. 2c), and LAI was still below 1 $\text{m}^2 \text{ m}^{-2}$ (Fig. 2d). Throughout winter (December 2022 ~~to~~ February 2023), N₂O fluxes remained near zero, ~~with daily means ranging from~~ (-0.1 to +0.9 $\text{nmol m}^{-2} \text{ s}^{-1}$). Following the first fertilization events ~~(on 27- and 28 February)~~, ~~providing a total of, which supplied~~ 111 kg N ha⁻¹ (total N; Table 1), N₂O fluxes increased sharply and exhibited three distinct peaks in March 2023. The first peak occurred shortly after fertilization, withreaching a daily mean flux of +6.2 $\text{nmol m}^{-2} \text{ s}^{-1}$ on 2 March

~~2023, under conditions of, with~~ topsoil WFPS above 65%, soil temperature below 5 °C, and LAI still below 1 m² m⁻². A second, larger peak followed approximately ten days later, reaching a daily mean flux of +13.6 nmol m⁻² s⁻¹ on 12 March and a maximum half-hourly flux (QC0) of +27.8 nmol m⁻² s⁻¹. ~~The last~~ A third, smaller peak occurred ~~between 25 and 29 at the end of~~ March, reaching ~~a daily mean flux of~~ +4.0 nmol m⁻² s⁻¹ on 28 March. These second and third peaks were preceded by precipitation events that raised topsoil WFPS above 80%, with soil temperature ranging from 5 to 10 °C, while LAI exceeded 1 m² m⁻² only during the last peak. ~~Following~~ After the ~~final~~ last fertilization ~~event~~ on 6 April (27 kg N ha⁻¹; Table 1), ~~net ecosystem~~ N₂O fluxes increased again, ~~with~~ reaching a daily mean ~~values reaching of~~ +5.1 nmol m⁻² s⁻¹ on 14 April 2023. ~~Although less pronounced than the March peaks, this emission event likewise followed rainfall that increased, under high topsoil~~ WFPS ~~above (≥ 80% (%; Fig. 2b), but occurred under) and~~ a more developed canopy, ~~with LAI being nearly double than that than~~ during the March peaks (Fig. 2d). During peak crop growth period, when LAI increased from 2.5 to 4 m² m⁻² (mid-April to late May; Fig. 2d), daily mean N₂O fluxes remained negligible (-0.4 to +1.4 nmol m⁻² s⁻¹), despite relatively high WFPS ~~values~~ (above 60% throughout the soil profile) and increasing soil temperatures. A short-lived emission event occurred after rewetting on 19 June, following ~~a drought~~ the dry period in May ~~and June 2023~~. Despite WFPS remaining below 40%, daily mean N₂O fluxes reached +11.2 nmol m⁻² s⁻¹ on 20 June, with a maximum half-hourly flux (QC0) of +21.6 nmol m⁻² s⁻¹, ~~at a time~~ when LAI was already declining ~~following~~ after anthesis ~~(Table A2)~~. In July, during ~~the final stages of late~~ wheat maturation and after harvest, ~~daily mean~~ N₂O fluxes remained low but positive (0.0 to +3.1 nmol m⁻² s⁻¹). A distinct peak occurred ~~in late July~~, shortly after ~~the cover crop was sown~~ sowing, with a daily mean flux of +7.3 nmol m⁻² s⁻¹ on 30 July. Emissions Fluxes remained low in August (0.0 to +2.3 nmol m⁻² s⁻¹) but ~~rose~~ increased slightly again following mulching of the cover crop and ~~subsequent~~ soil cultivation tillage in late September 2023.

3.2.3 ~~Net ecosystem~~ CH₄ fluxes

~~Net~~ CH₄ fluxes remained low throughout the measurement period, typically indicating small CH₄ emissions, with daily average fluxes ranging from -7.0 to +28.5 nmol CH₄ m⁻² s⁻¹ (Fig. 3c). ~~No consistent temporal patterns were evident, although slightly elevated fluxes indicating net CH₄ release were recorded from mid-October to early November 2022 and in early January 2023 (Fig. 2). Higher CH₄ emissions occurred from mid-October to early November 2022 as well as in January 2023, while weak CH₄ uptake occurred during the dry period in May and June. The mean measured CH₄ flux during the measurement period was +0.77 ± 8.57 nmol CH₄ m⁻² s⁻¹, with a median signal-to-noise ratio of 1.55, calculated as the flux record divided by its random uncertainty (estimated following Finkelstein and Sims, 2001), indicating weak net CH₄ exchange that was only marginally distinguishable from measurement noise.~~

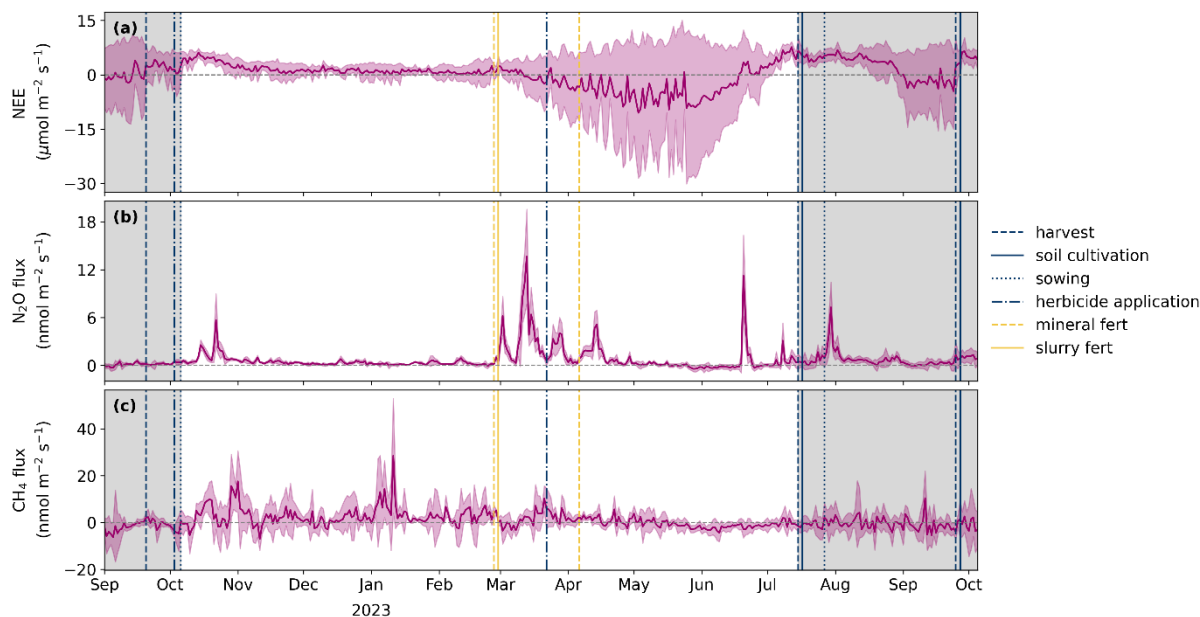


Figure 3. Gap-filled greenhouse gas fluxes at the Oensingen cropland measured from September 2022 to October 2023. The unshaded area corresponds to the winter wheat cropping season, while the shaded areas indicate the final phase of the preceding temporary grassland and the cover crop following winter harvest. (a) Net ecosystem CO₂ exchange (NEE), (b) ~~net-ecosystem~~-N₂O fluxes, and (c) ~~net-ecosystem~~-CH₄ fluxes. Fluxes were gap-filled using the Marginal Distribution Sampling (MDS) for NEE and random forest (RF) for N₂O and CH₄ fluxes. Lines represent daily averages of the gap-filled half-hourly fluxes, while the shading indicates ± 1 standard deviation. Vertical lines mark management activities: yellow dashed = mineral fertilization (fert), yellow solid = slurry fertilization (fert), blue solid = soil cultivation, blue dotted = sowing, blue dashed = harvest, and blue dash-dot = herbicide application. See Table 1 for details on management activities.

3.3 ~~N₂O emission factor and~~ Net greenhouse gas budget~~exchange and net GHG budget~~

During the winter wheat cropping season (282 days), cumulative N₂O emissions were 5.5 kg N₂O-N ha⁻¹ (Table 2), with an average gap-filled flux of 0.81 nmol m⁻² s⁻¹. When scaled to crop yield, this corresponded to 1.1 kg of N₂O-N emitted per ton of wheat grain (dry matter). ~~A background N₂O flux of 0.44 nmol m⁻² s⁻¹ was calculated as the average of gap filled fluxes outside the 30-day post fertilization periods, thereby minimizing the influence of short term fertilization induced peaks. Accounting for this background flux, the N₂O-cumulative flux due to fertilization induced emissions amounted to 2.5 kg N₂O-N ha⁻¹ during the winter wheat cropping season, accounting for approximately 45% of~~ Based on the total N₂O emissions. Based on a total-N input from fertilizers of 138 kg N ha⁻¹ (Table 1), the resulting apparent emission factor (EF) was 4.0%. ~~Over the one-year period starting at winter wheat sowing, cumulative N₂O emissions amounted to 7.0 kg N₂O-N ha⁻¹, corresponding to an annual apparent EF of 5.1-8%.~~ Because no unfertilized control treatment was available, both values include N₂O emissions that cannot be attributed uniquely to fertilizer application. During the subsequent 60-day cover crop season, cumulative N₂O emissions reached 1.1 kg N₂O-N ha⁻¹, and the average daily sum of N₂O emissions (17.6 g N₂O-N ha⁻¹ d⁻¹) was only slightly lower than that observed during the winter wheat season (19.6 g N₂O-N ha⁻¹ d⁻¹).

Throughout the winter wheat cropping season, the ecosystem acted as a net CO₂ sink, with a cumulative NEE of -89 g CO₂-C m⁻² (Table 2). ~~However, this climate benefit was largely offset (-70%) by~~ When expressed in CO₂-equivalents, concurrent ~~net~~-N₂O emissions ~~offset approximately 70% of this seasonal net CO₂ uptake~~, while ~~net~~-CH₄ emissions remained negligible. The resulting net GHG exchange (NGHGE) was therefore slightly negative, representing a small GHG sink with -76 g CO₂-eq m⁻². In contrast, the ~~short summer~~ cover crop ~~acted as a period represented~~ a net CO₂ source, emitting 108 g CO₂-C m⁻². ~~Net~~ N₂O emissions during this period accounted for approximately 10% of ~~the total GHG budget, NGHGE~~, while the net CH₄ ~~sink exchange~~ was again negligible. ~~The difference in NEE between the two crops was reflected in their respective GHG budgets: winter wheat resulted in a~~ The NGHGE during the cover crop period showed large net GHG sink of -76 g CO₂-equivalents (CO₂-eq) m⁻², while the cover crop resulted in a net GHG source of emissions (+441 g CO₂-eq m⁻²). The difference between the two crops was even more ~~striking~~pronounced when comparing their daily ~~sums of CO₂-eq~~NGHGE, with winter wheat averaging -0.27 g CO₂-eq m⁻² d⁻¹ and the cover crop averaging +7.4 g CO₂-eq m⁻² d⁻¹, resulting in a daily difference of approximately 8 g CO₂-eq m⁻² d⁻¹ (Table 2). ~~However, when lateral C fluxes were included to calculate the net GHG budget, winter wheat was a substantial net GHG source (+1349 g CO₂-eq m⁻²), due to its large C export with harvested grain and straw, while the cover crop was a smaller net GHG source (+441 g CO₂-eq m⁻²; note: numbers are identical to NGHGE because no lateral C fluxes occurred). Sensitivity analysis across alternative u_e thresholds (CUT16, CUT84) showed a NGHGE spread of 82 g CO₂-eq m⁻² for winter wheat versus 26 g CO₂-eq m⁻² for the cover crop, driven mainly by~~ CO₂ fluxes (Table A3).

Table 2. Cumulative greenhouse gas (GHG) fluxes, net GHG exchange (NGHGE), lateral C fluxes, and daily average sums net GHG budget for the winter wheat and ~~the cover crop~~ cropping seasons (282 and 60 days, respectively), ~~shown separately for~~. NGHGE represents the three-gases EC-based sum of CO₂, N₂O, and CH₄, as well as the GHG budget (sum of all three gases). No fluxes, expressed in CO₂-equivalents. The net GHG budget additionally includes lateral C inputs or from organic fertilizer and C exports (fertilization, with harvest) are included in the flux budget. (grain and straw), with all fluxes converted to CO₂-equivalents using the molecular mass ratio of CO₂ to C. Negative values indicate net uptake, while or C input to the ecosystem, whereas positive values ~~represent indicate~~ net release of CO₂, N₂O, and CH₄ to the atmosphere or C export. CO₂-equivalents (g CO₂-eq m⁻²) for N₂O and CH₄ were calculated using global warming potentials (GWP₁₀₀) of 273 and 27, respectively, applied to fluxes expressed in g m⁻² (IPCC, 2021).

		Winter wheat (282 days)	Cover crop (60 days)
CO ₂	Cumulative (g CO ₂ -C m ⁻²)	-89	+108
	Cumulative (g CO ₂ -eq m ⁻²)	-329	+397
	Daily (g CO ₂ -eq m ⁻² d ⁻¹)	-1.17	+6.62
N ₂ O	Cumulative (kg N ₂ O-N ha ⁻¹)	+5.5	+1.1
	Cumulative (g CO ₂ -eq m ⁻²)	+237	+45
	Daily (g CO ₂ -eq m ⁻² d ⁻¹)	+0.84	+0.76
CH ₄	Cumulative (g CH ₄ -C m ⁻²)	+0.45	-0.03
	Cumulative (g CO ₂ -eq m ⁻²)	+16	-1
	Daily (g CO ₂ -eq m ⁻² d ⁻¹)	+0.06	-0.02

Net GHG exchange	Cumulative (g CO ₂ -eq m ⁻²)	-76	+441
	Daily (g CO ₂ -eq m ⁻² d ⁻¹)	-0.27	+7.35
Lateral C fluxes			
Fertilizer C	Cumulative (g C m ⁻²)	-48	0
Harvest C	Cumulative (g C m ⁻²)	+437	0
Net GHG budget	Cumulative (g CO ₂ -eq m ⁻²)	+1349	+441
	Daily (g CO ₂ -eq m ⁻² d ⁻¹)	+4.8	+7.35

3.4 Drivers of N₂O flux dynamics over time

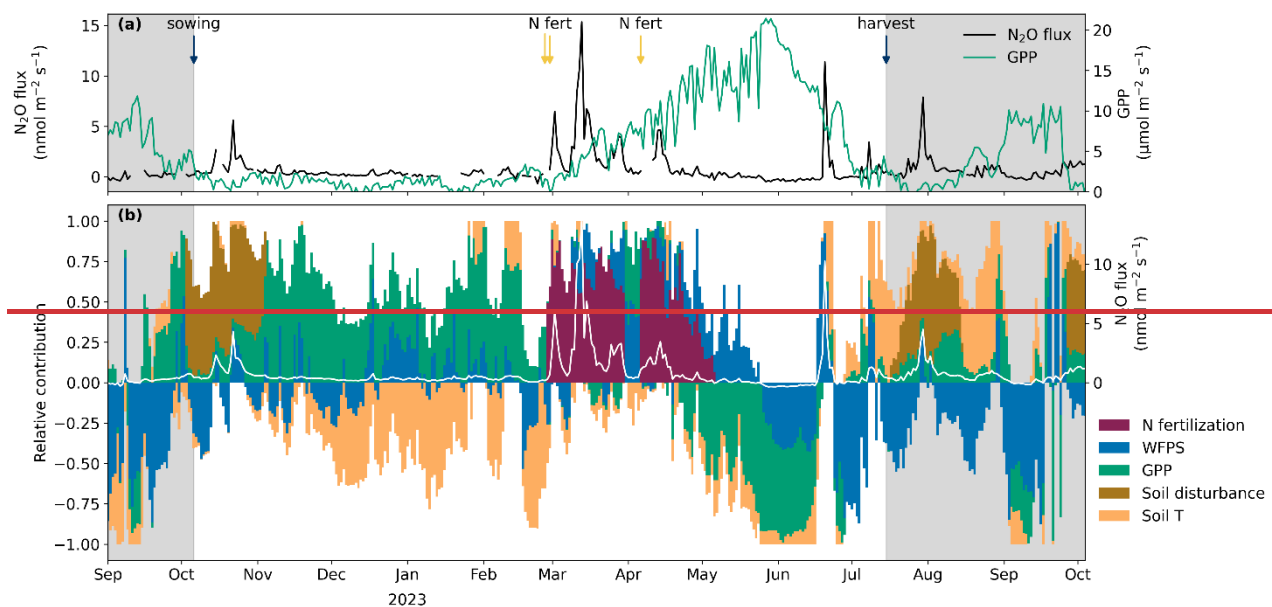
3.4.1 Temporal development of N₂O flux driver contributions

We used SHAP to quantify both the magnitude and direction (positive or negative) of each driver's contribution to ~~net~~
ecosystem-N₂O fluxes across ~~all three crops, the measurement period,~~ relative to a ~~reference state~~ (baseline). ~~In our case, the~~
~~. The SHAP~~ baseline ~~represents and thus~~ the ~~model's corresponding~~ expected N₂O flux ~~under rather undisturbed conditions~~
~~(avoiding post-, when 30 days after fertilization and post-soil management periods) and preparation were excluded,~~ was
estimated ~~as at~~ 0.2745 nmol N₂O m⁻² s⁻¹ ~~using a subset of the data (see Sect. 2.7.2). This baseline value was lower than the~~
~~N₂O background flux given above, since we also excluded post-soil management periods.~~ To assess the overall influence of
each driver across the study period, we summed up the SHAP values over time, ~~but~~ separately for positive and negative
contributions. This approach avoided cancelling out opposing effects and revealed how strongly each driver enhanced or
decreased N₂O emissions (Fig. A3). N fertilization and soil disturbance increased the N₂O fluxes (i.e., positive SHAP values)
relative to the baseline. In contrast, soil moisture, soil temperature, and GPP exhibited both positive and negative SHAP
values, reflecting their capacity to either increase or decrease N₂O fluxes depending on environmental conditions. Across the
study period (September 2022 ~~to~~ October 2023), N fertilization was the dominant driver increasing N₂O fluxes (~~3743%~~ of
all positive contributions), while soil moisture (~~2319%~~), GPP (17%), soil disturbance (~~16%~~), ~~GPP (1412%)~~, and soil
temperature (~~109%~~) also contributed to positive deviations from the baseline flux. Conversely, soil moisture (~~4841%~~ of all
negative contributions), GPP (30%), and soil temperature (~~28%~~), ~~and GPP (2429%)~~ showed substantial negative
contributions, indicating periods when these variables reduced N₂O fluxes relative to the baseline. SHAP dependence plots
further showed that high recent N input, short time since fertilization or since soil preparation, high-WFPS episodes, and
warmer soil conditions were generally associated with positive SHAP values (Fig. A4).

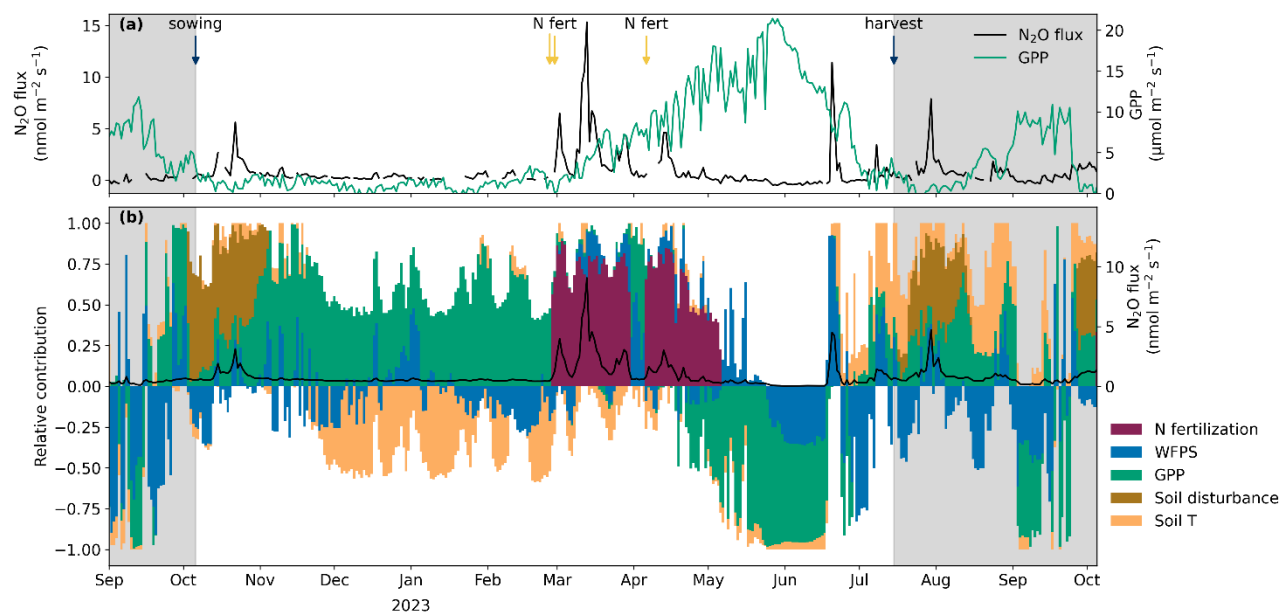
To assess the relative influence of each driver in a time-resolved manner and independently of the absolute magnitude of
predictions, we computed daily averages of normalized SHAP values (see Sect. 2.7.2). These relative driver contributions
revealed distinct temporal patterns across the study period (September 2022 ~~to~~ October 2023; Fig. 4). In September 2022,
during the final grassland regrowth phase, N₂O emissions were mainly suppressed by WFPS (negative relative contributions;
Fig. 4), although GPP exerted a positive effect later in the month. At the beginning of October, herbicide application and the

direct seeding of wheat introduced soil disturbance, and N₂O fluxes during crop establishment were primarily driven by soil disturbance and GPP (positive relative contributions; Fig. 4). Throughout winter (November 2022 ~~-to~~ February 2023), soil temperature consistently suppressed N₂O emissions ~~-(negative relative contributions),~~₂ while GPP maintained a positive effect. In spring (March ~~-to~~ April 2023), which corresponded to the period of highest observed N₂O fluxes (Fig. 4a), emissions were primarily driven by N fertilization, followed by WFPS. Later in the season, when photosynthetic activity and presumably plant N demand increased (April), the effect of GPP shifted towards decreasing N₂O fluxes. The low N₂O emissions observed from May to mid-~~to~~ June were thus strongly driven by large negative effects of ~~soil temperature, GPP,~~ and WFPS (Fig. 4b). In contrast, during grain filling and post-harvest (July to mid-August), the SHAP analysis indicated that soil temperature ~~and,~~ soil disturbance ~~strongly, and GPP~~ increased N₂O emissions, ~~while GPP had a smaller but still positive effect.~~ Following the establishment of the cover crop in September, the effect of GPP became negative again, coinciding with an increase in photosynthetic CO₂ uptake.

~~To investigate the changing role of GPP in more detail, we focused on the winter wheat period from March 2023 to harvest (mid July 2023), thereby limiting potential confounding factors (Fig. 5). In this period, N₂O fluxes were negatively related to GPP, suggesting that high photosynthetic activity (high GPP) was associated with low N₂O emissions. This relationship was modulated by WFPS: the decline in N₂O fluxes with increasing GPP was weakest in the driest WFPS class ($\leq 55\%$) and became progressively stronger at higher soil moisture, as indicated by increasingly negative regression slopes ($R^2 = 0.28, 0.62, \text{ and } 0.80$; all $p < 0.001$; Fig. 5).~~



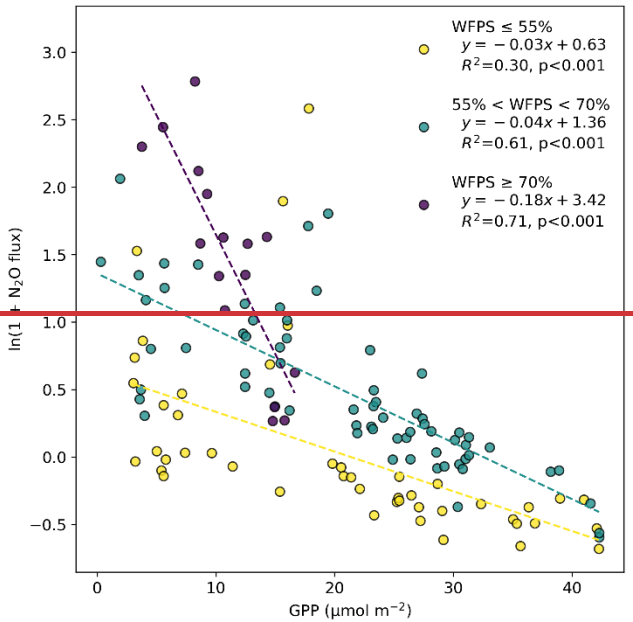
640 The SHAP dependence plot for GPP showed a clear shift from mostly positive SHAP values at low GPP to increasingly negative SHAP values at higher GPP (Fig. 5). Thus, low crop activity was generally associated with higher predicted N_2O fluxes, whereas periods of greater crop activity were associated with lower predicted N_2O fluxes.



645 **Figure 4. Temporal dynamics of N_2O fluxes, gross primary productivity (GPP), and relative driver contributions to N_2O fluxes at the Oensingen cropland from September 2022 to October 2023. The unshaded area corresponds to the winter wheat cropping season, while the shaded areas indicate the final phase of the preceding temporary grassland and the cover crop following winter harvest. (a) Daily average N_2O fluxes (measured, highest quality fluxes only) are shown in black, and daily average GPP in green. Arrows at the top denote management activities conducted during the winter wheat cropping season. (b) Relative contributions of**

650

individual drivers (i.e., N fertilization, water-filled pore space (WFPS), GPP, soil disturbance, and soil temperature (soil T)) are expressed as daily averages of normalized SHAP values (see Sect. 2.67.2 for methodological details). The baseline (SHAP = 0) corresponds to a predicted N₂O flux of 0.2745 nmol m⁻² s⁻¹. Positive values indicate a driver's increasing effect on N₂O fluxes, while negative values reflect a decreasing effect. The whiteblack line represents the model-predicted N₂O flux.



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Figure 5. Relationship between gross primary productivity (GPP; rolling sum over the preceding 48 h) and the measured N₂O fluxes (QC0 only, daily averages) between March and mid-July 2023 in winter wheat. Points are colored by water-filled pore space classes (WFPS; at 0.3 m soil depth), based on the 48 h rolling mean of WFPS (same window as for GPP). Dashed lines show the linear regressions for each class, with the corresponding regression statistics given as well.

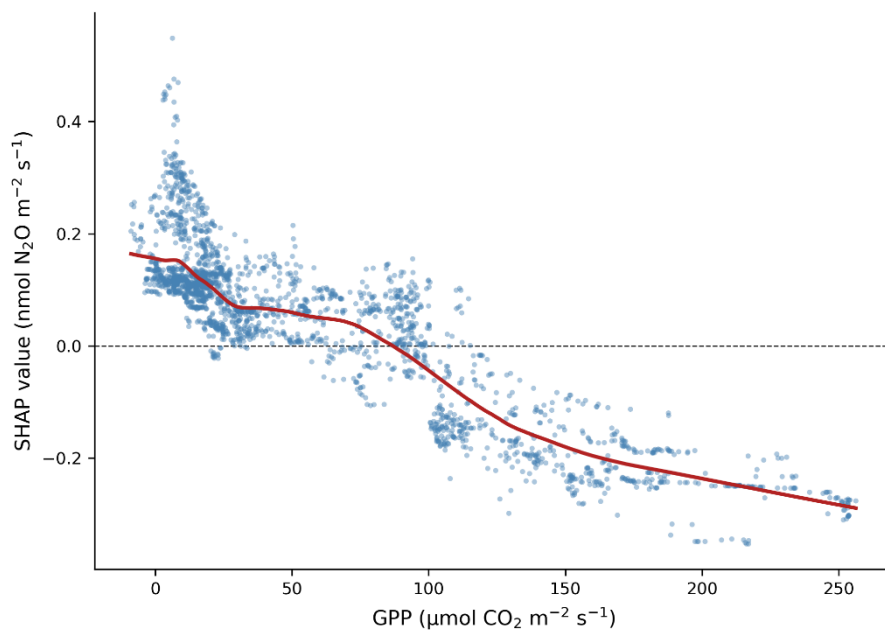


Figure 5. SHAP dependence plot showing the SHAP value of GPP (rolling sum over the preceding 48h) against its observed values across all data, reflecting GPP's marginal contribution to the modelled N₂O fluxes. A LOWESS smoother (red line) is overlaid to highlight the overall trend.

3.4.2 Soil available nitrogen

To assess soil N availability to roots and microorganisms, we used two complementary approaches: (i) time-integrated supply of plant-available NO₃⁻-N measured with PRS probes, and (ii) instantaneous mineral N supply pools (N_{min}), derived from soil-extractable NO₃⁻ and NH₄⁺ concentrations in the 0-0.3 m soil layer. N₂O fluxes increased significantly with soil mineral N availability, both for integrated (Fig. 6c, R² = 0.61; p<0.05) and instantaneous supply (Fig. 6d; R² = 0.77; p<0.05). The lowest N₂O emissions occurred during periods of highest GPP (point 4 in Fig. 6c; point D in Fig. 6d) or without prior fertilization events (points A and B in Fig. 6d). In contrast, the highest N₂O emissions occurred after fertilization events, when soil mineral N availability was highest (points 1 and 2 in Fig. 6c; point C in Fig. 6d), with average N_{min} values reaching 74 kg N ha⁻¹ ten days after the first fertilization. Between these extremes, intermediate N availability was observed in December 2022 (point A in Fig. 6d) and in August 2023 during the post-harvest period (points 6 and 7 in Fig. 6c; point E in Fig. 6d). While in August the intermediate N availability coincided with higher N₂O emissions, this was not the case in December, when soil temperature at 0.05 m depth ranged between 3 and 5 °C during the sampling week.

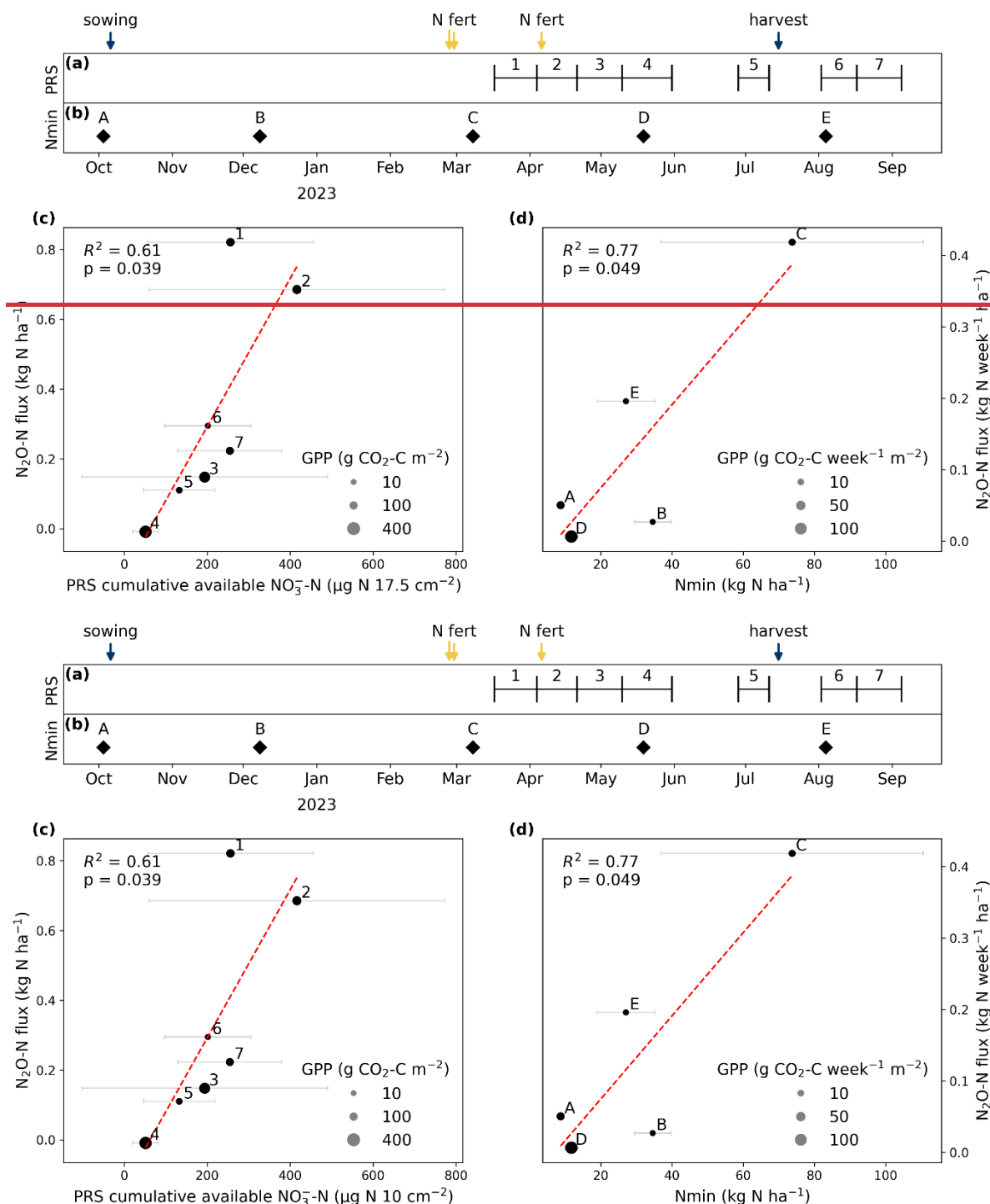


Figure 6. Relationships between nitrogen (N) availability and N₂O fluxes. (a) Timeline of burial periods for plant root simulators (PRS) probes, and (b) of soil mineral N (N_{min}) sampling campaigns. Sowing, harvest, and fertilization dates are also provided. (c) Relationship between cumulative available NO₃⁻-N (μg N 17.5 cm⁻², based on PRS probes) and cumulative N₂O fluxes over the

680 corresponding burial period (15 to 21 days). Means and ± 1 standard deviation are given (n=5). Circle size reflects cumulative
GPP during the same period. Numbers indicate the corresponding period as shown in panel (a). A linear regression is shown as a
dashed red line, together with the coefficient of determination (R^2) and corresponding p-value. (d) Relationship between $N_{\min}$ (0-
0.3 m soil depth) and cumulative N_2O fluxes during the week centered on the soil sampling (± 3.5 days). Means ± 1 standard
deviation are given (n= 4; except for 1st sampling with no replicates). Circle size reflects cumulative GPP during the same period.
685 Letters indicate the corresponding period as shown in panel (b). A linear regression is shown as a dashed red line, together with
the coefficient of determination (R^2) and corresponding p-value.

3.5 ~~N₂O sources using~~producing processes inferred from stable isotopes

We used stable oxygen and nitrogen isotopes to identify the microbial processes underlying the measured N₂O fluxes: ~~during the three weeks following the first fertilization events on 27 and 28 February 2023.~~ The $\delta^{18}\text{O}$ ~~and site preference (SP-N₂O) of emitted~~ N₂O ranged between 17.3 and 39.8‰, ~~while the site preference (SP-N₂O) ranged‰ and~~ from -7.2 to +18.2‰‰, ~~respectively~~ (Fig. 7a). The dual isotope plots suggested that heterotrophic bacterial denitrification and/or nitrifier denitrification were the dominant N₂O production pathways ~~during the three weeks following the fertilization events on 27 and 28 February 2023 (Fig. Fig. 7a; Fig. A5).~~ Moreover, the observed trend of increasing enrichment of $\delta^{18}\text{O}$ and SP-N₂O over time (Fig. 7a) suggested isotopic fractionation associated with the microbial reduction of N₂O to N₂ during denitrification. Results from the FRAME model supported the qualitative source attribution derived from the isotopic ~~ie~~ mapping approach and enabled the quantification of both the relative contributions of individual N₂O -producing processes- ~~and the extent of N₂O reduction to N₂.~~ However, following Buchen et al. (2017), we pooled heterotrophic bacterial denitrification with nitrifier denitrification, and nitrification with fungal denitrification, due to the large uncertainty in separating these processes given their similar endmembers. All four processes are nonetheless shown separately in Fig. A6. While N₂O fluxes slowly decreased over time (Fig. 7b), the contributions of these processes ~~also~~ slightly changed over time. ~~Heterotrophic~~ bacterial denitrification and nitrifier denitrification together ~~accounted for approximately 90% of~~ dominated N₂O production ~~(Fig. 7c), except throughout the sampling period, contributing 78 ± 15% on 1 March, when and 86-90% (±7-8%) on the subsequent sampling dates (Fig. 7c; based on the mixing-reduction scenario).~~ Nitrification and/or fungal denitrification contributed ~~up to 2022 ± 15% of the total. Moreover, the gradual increase of N₂O production on 1 March, and declined thereafter. The alternative reduction-mixing scenario yielded very similar source fraction distributions, not changing the overall interpretation (Fig. A6).~~ The reduced N₂O-fraction, reported as (1 - r), increased over time ~~(Fig. 7c) indicated, indicating a shift toward more complete denitrification, which coincided with a decrease in larger fraction of N₂O reduced to N₂ during the later sampling dates, coinciding with decreasing chamber-based~~ N₂O fluxes (Fig. 7b).

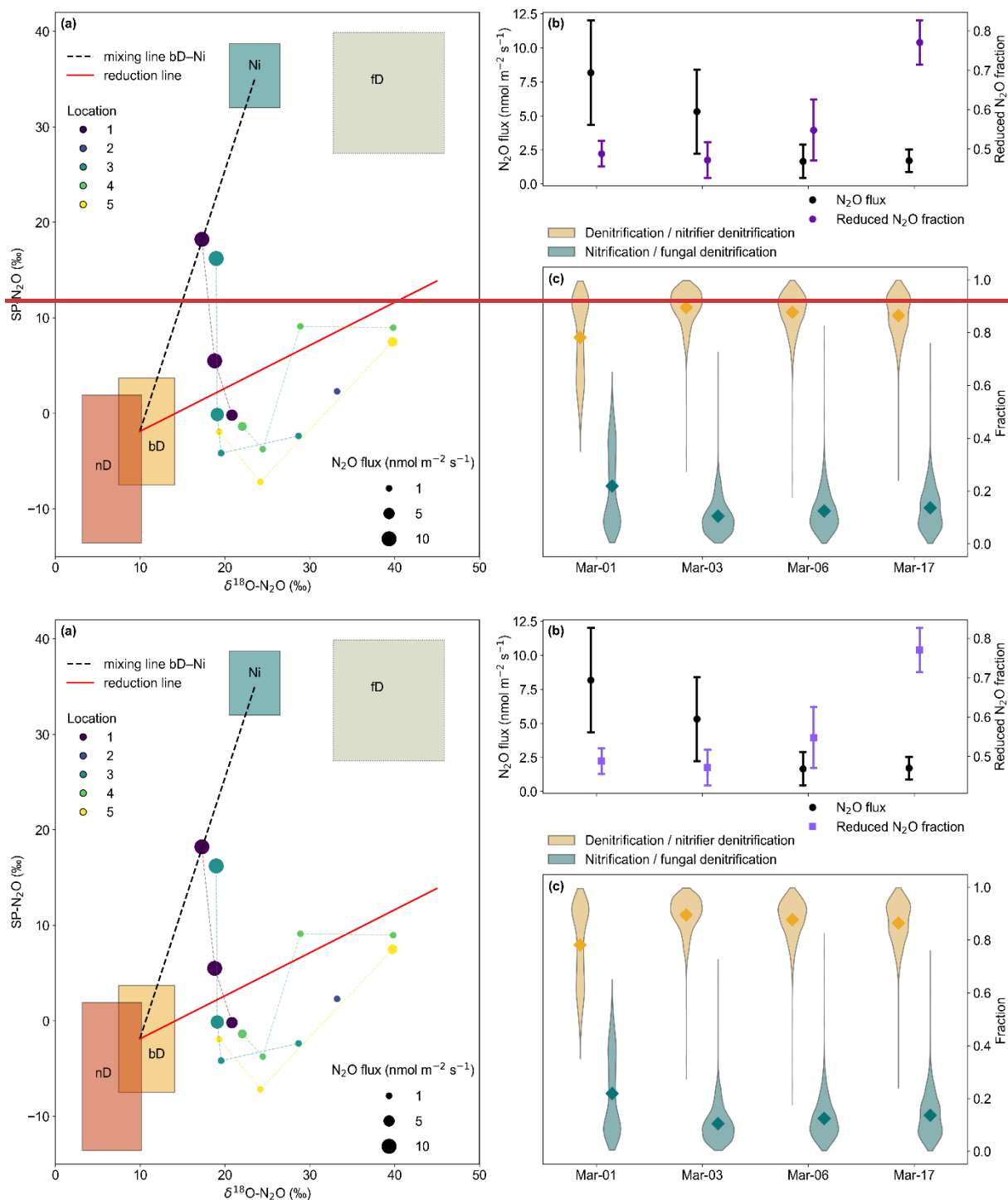


Figure 7. Isotopic signature of N_2O , N_2O flux magnitudes, and their estimated source fractions in March 2023, following fertilization applied on 27 February (ammonium-nitrate) and 28 February (slurry). (a) Dual isotope plot of $\delta^{18}\text{O-N}_2\text{O}$ vs. site preference (SP- N_2O). Colored boxes denote endmembers for the N_2O mixing (nD: nitrifier denitrification, bD: heterotrophic

bacterial denitrification, Ni: nitrification, fd: fungal denitrification). Endmember values of boxes are derived from Yu et al. (2020) and adjusted to the values of soil water ($\delta^{18}\text{O}\text{-H}_2\text{O} = -9.2\text{‰}$) at the study site (except for the Ni box). Lines for mixing (black) and N_2O reduction to N_2 (red) are shown. Individual measurements are shown as circles, with size reflecting flux magnitude and color indicating location (1 to 5; see Fig. 1). (b) N_2O fluxes measured with static chambers (black) and the fraction of N_2O reduced N_2O fractions to N_2 estimated by the FRAME model (purple). The latter is expressed as $(1 - r)$, where r denotes the residual unreduced N_2O fraction. Values represent means $\pm$ one standard error across measurement locations. (c) N_2O source fractions estimated by the FRAME model, based on the mixing-reduction scenario, for heterotrophic bacterial denitrification & nitrifier denitrification and nitrification & fungal denitrification, displayed as violin plots, with mean values indicated by diamonds (see text for details).

4. Discussion

4.1 ~~Seasonal changes in~~ Explainable machine learning for analysing N_2O fluxes and their drivers flux dynamics

~~The~~ Two central ~~aim~~ objectives of this study ~~was~~ were to quantify N_2O fluxes and determine *when* and *how* ~~different~~ biophysical–environmental and management ~~factors influenced N_2O –drivers affected these~~ fluxes during a winter wheat cropping season, ~~to uncover seasonal patterns in– and the contributions of each driver.~~ Two periods emerged as particularly sensitive to net N_2O emissions: crop establishment and early spring. Elevated N_2O emissions during the establishment phase of winter wheat were primarily driven by soil disturbance and low GPP. Low GPP reflected limited plant N uptake, while soil disturbance, resulting from subsequent cover crop season. To address these objectives, we used an explainable ML framework (i.e., XGBoost-SHAP) as an interpretative tool to extract, from high-frequency EC observations, the temporal development of driver contributions to N_2O fluxes. We chose this approach over traditional statistical models for three reasons. First, N_2O fluxes are highly episodic and respond non-linearly to interacting drivers, conditions under which ML models are expected to outperform linear models (Gnisia et al., 2025; Hamrani et al., 2020). Second, SHAP values allowed us to quantify not only the average importance of each driver, but also how its contribution evolved over time. Third, this framework let us incorporate management history alongside continuous biophysical drivers, enabling interpretation of management effects not possible with classical statistical analyses. As with any data-driven approach, these advantages come with trade-offs: SHAP quantifies how each driver contributes to the model's predictions rather than establishing process-based causal effects, and the framework benefits from large datasets to constrain overfitting. In our study, however, high-resolution environmental and EC data over a full year provided a reliable basis for this approach: the XGBoost model captured the temporal patterns of N_2O fluxes well, though it underestimated high peaks and overestimated low fluxes (Fig. A2), and the resulting SHAP attributions were consistent with established process understanding and published field studies (see below), supporting a mechanistic rather than spurious interpretation of the identified drivers. Integrating ML with process-based models (Saha et al., 2021; Sharma et al., 2026) or adopting knowledge-guided ML approaches (Liu et al., 2022) are promising next steps to address the complexity of N_2O emissions from managed ecosystems.

4.2 Seasonal changes in N₂O fluxes and their drivers

Two periods emerged as particularly relevant for N₂O emissions: crop establishment and early spring. Both were characterized by a mismatch between N supply and plant demand, with substantial mineral N supply from mineralization or fertilization coinciding with limited crop uptake, resulting in surplus soil mineral N, that under favorable moisture and temperature conditions, fuelled microbial N₂O production.

During crop establishment, elevated emissions were affected by soil disturbance and low crop activity (i.e., low GPP). Herbicide termination of the temporary grassland and direct seeding of winter wheat, likely stimulated mineralization of soil organic matter and crop residues. ~~This was supported by an increase in net ecosystem exchange of CO₂ (NEE), indicating, as indicated by increased NEE (intensified soil respiration. Furthermore,)~~, while low GPP reflected limited plant N uptake (Fig. A1). Together, these processes raised soil N_{min} ~~increased from 8.7 kg N ha⁻¹ before crop seeding to 34.6 kg N ha⁻¹ by between October and~~ early December 2022 (0-0.3 m soil depth; Fig. 6d), ~~indicating elevated N availability due to low plant N uptake and enhanced N mineralization, consistent with previous consistent with~~ observations after ~~herbicidegrassland~~ termination of grassland swards from (Buchen et al. (., 2017) and; Helfrich et al. (., 2020). A ~~similar pattern was also observed comparable response occurred~~ during cover-crop establishment after wheat harvest: ~~although wheat residues had a lower N concentration (%N) than grassland residues (including clover), elevated soil temperature and mechanical disturbance during post harvest operations likely,~~ when warm soil temperatures and soil tillage enhanced mineralization of soil organic matter (Grandy and Robertson, 2006). ~~This was supported by an increase in soil-) and N_{min} rose from 12 kg N ha⁻¹ in late May to 27 kg N ha⁻¹ in between late May and~~ early August (0-0.3 m soil depth; Fig. 6d). Thus, different management practices leading to no or reduced vegetation performance favor N₂O emissions.

~~The high that left soils disturbed and poorly vegetated favored~~ N₂O emissions ~~in early spring,~~ and mitigation in these phases will depend on promoting rapid and sustained crop growth, e.g., through optimized sowing dates and cultivar choice (Maier et al., 2025; Tallec et al., 2022).

In early spring, high N₂O emissions were predominantly driven by N fertilization, with WFPS contributing significantly during peak ~~emission events, while GPP consistently decreased emissions from mid April onward.~~ The first fertilizer applications in late February ~~supplied combined mineral (NH₄NO₃) and organic (slurry) N, supplying a large N input (111 kg N ha⁻¹) during the early crop development stage (at tillering) and, which~~ coincided with high soil moisture, conditions typical ~~offor~~ central European climates (Ruosteenoja et al., 2018). At this stage, ~~both low~~ LAI (Fig. 2d) and ~~photosynthetic CO₂ assimilation rates low GPP (Fig. 4a) were still low, indicating indicated~~ limited plant N uptake typical of early growth stages in Swiss winter wheat systems (Argento et al., 2022). These conditions resulted in excess N availability, ~~with demand, so that~~ soil N_{min} ~~reaching~~ 74 kg N ha⁻¹ (0-0.3 m soil depth; Fig. 6d), which, ~~in combination together~~ with precipitation events ~~that increased WFPS (Fig. 2b2a),~~ created optimal conditions for microbial N₂O production. By contrast, the ~~final fertilization in early April 2023 involved a smaller N input final application in early April (27 kg N ha⁻¹) and was timed to coincide with the done during~~ stem elongation phase, when plant N demand is typically very high. This is supported

by, when higher LAI ($\sim 2 \text{ m}^2 \text{ m}^{-2}$; Fig. 2d) and higher GPP (Fig. 4a), indicative of active growth and greater N assimilation. Under these conditions, less mineral N was likely available for microbial activity, indicated high plant N demand, likely reducing substrate availability for N_2O production and resulting in significantly lower N_2O losses.

Over the entire study period, nitrogen (N). Mitigation in this phase will depend on better synchronizing fertilizer N inputs with crop demand and soil N mineralization through adjusted timing and amounts (Hoben et al., 2011; Omonode et al., 2017), split applications, site-specific planning (Jordan-Meille et al., 2023), precision fertilization emerged as (Diacono et al., 2013) or enhanced-efficiency fertilizers (Akiyama et al., 2010).

Over the study period, N fertilization was the dominant positive driver of increasing N_2O fluxes (Fig. A3), consistent with its role as the primary source of reactive nitrogen in croplands (Shcherbak et al., 2014). However, substantial and temporally dynamic contributions of soil moisture (WFPS), gross primary productivity (GPP), soil temperature, and soil disturbance highlighted made substantial but temporally varying contributions, underlining the multifactorial and interactive nature of N_2O emissions and the need to consider both biophysical and management drivers, along with their complex interactions. Overall, WFPS exhibited, WFPS had both positive and negative effects, but consistently emerged as a key driver during peak N_2O -emission events. GPP, used here as a proxy for crop N uptake, showed a clear negative relationship with N_2O fluxes: low GPP was activity and N demand, was negatively associated with elevated N_2O emissions, while sustained photosynthetic activity decreased emissions fluxes (Fig. 5). This supported earlier observations that active crop growth competes with We interpreted this result as an indirect, plant-mediated effect, reflecting microbial processes for substrate limitation: as the crop grows, its N uptake depletes soil mineral N available N, thereby limiting for microbial N_2O production (Abalos et al., 2018; Feigenwinter et al., 2023; Maier et al., 2022; Timilsina et al., 2024). Further evidence was found in the observed decline in soil N availability. Because WFPS was included in the model, an alternative pathway, i.e., high transpiration rates lowering soil moisture and thereby suppressing N_2O production, was already accounted for. Although root C exudation might favor denitrification (Philippot et al., 2009), the negative relationship suggests substrate limitation dominated. Consistent with this explanation, soil N availability declined during periods of high GPP, particularly in late May (Fig. 6), suggesting efficient crop N uptake. Interestingly, the limiting effect of GPP on N_2O fluxes appeared to be strongly modulated by soil moisture, with larger limitations, i.e., steeper negative slopes observed under higher WFPS conditions (Fig. 5). This provided additional evidence that plant N uptake plays a critical role in mitigating emissions under environmental conditions favorable for N_2O production.

4.2 N_2O emission factor and greenhouse gas budgets

In this study, an EF of 1.8% was estimated for winter wheat, slightly exceeding the IPCC (2019) default value of 1.6% for synthetic N fertilizers in wet climates (Table 2). However, in our study, approximately 30% of the applied N was derived from organic fertilizer applied as slurry, for which the IPCC recommends a lower EF of 0.6%. When accounting for the mixed N sources, the weighted IPCC default EF for 6). Overall, our cropping system is 1.3%, indicating results support the 'N synchrony framework', originally suggested by Cassman et al. (2002) and revisited by Cassman and Dobermann in 2022.

While the original concept aimed to increase crop N use efficiency by synchronising N supply with crop N demand, our study expands this framework to N₂O emissions, showing that the observed EF exceeded this value by 0.5 percentage points. such synchronisation can lower N₂O losses, representing an easy-to-implement N₂O mitigation option.

4.3 Cumulative N₂O losses and net GHG exchange

815 Cumulative N₂O emissions during the winter wheat season were 5.5 kg N₂O-N ha⁻¹, substantially exceeding the ranges reported for winter wheat by Garnier et al. (2024) for northern France (0.1 - 2.7 kg N₂O-N ha⁻¹) and by Tallec et al. (2022) for southwestern France (0.95 - 2.91 kg N₂O-N ha⁻¹), both ~~studies using chamber measurements-based studies~~, although our N input (138 kg N ha⁻¹) was well within their ~~input reported fertilizer~~ ranges. Yield-scaled N₂O emissions in our study (1.1 kg N₂O-N Mg⁻¹ grain) were approximately three times higher than ~~the global wheat values reported for wheat~~ by Yao et al. 820 (2024) ~~(; 0.301 - 0.346 kg N₂O-N Mg⁻¹). These discrepancies may partly reflect grain~~. Part of this discrepancy is likely methodological ~~differences, as, since global meta-analyses predominantly compile chamber-based flux measurements, which typically have lower temporal and syntheses rely largely on soil chambers with lower spatial resolutions than the continuous EC flux measurements used in our study.~~ High frequency EC measurements are valuable for capturing short-lived N₂O emission peaks and for integrating the highly dynamic N₂O fluxes over a larger spatial area and temporal coverage 825 ~~than chamber measurements. Despite higher equipment costs and computational requirements, EC measurements thus improve the representativeness and the accuracy of cumulative N₂O loss estimates.~~ continuous EC, which better captures short-lived peaks and integrates fluxes over larger areas. Beyond methodology, the elevated emissions may partly reflect site-specific management: the near-simultaneous application of mineral N and slurry at the end of February likely created conditions particularly conducive to N₂O production, owing to the input of readily degradable carbon (Dittert et al., 2005; 830 Schils et al., 2008).

To our knowledge, this is the first study to report EC-based N₂O fluxes over a complete winter wheat ~~cropping~~ season. Notably, our N₂O emissions from winter wheat only slightly exceeded those observed for maize in Switzerland (with EC: 4.8 kg N₂O-N ha⁻¹; Maier et al., 2022), despite ~~at the much shorter cropping season of maize season (127 days) compared to that of winter wheat (vs 282 days; about 2.2 times longer).~~. The two crops also clearly differed in their N use efficiency (NUE), 835 calculated as the ratio between N output to N input, ~~with not accounting for soil N mineralisation~~; winter wheat ~~taking took~~ up ~~162~~113 kg N ha⁻¹ from an input of 138 kg N ha⁻¹ (NUE ~~=117~~of 82%), whereas maize took up only 56 kg N ha⁻¹ from an input of 110 kg N ha⁻¹ (NUE ~~=of 51~~%) ~~%; derived from Table 1 in Maier et al., 2022~~. The higher wheat NUE ~~observed for wheat~~ is consistent with ~~findings from~~ Yu et al. (2022) and ~~can be due to many factors, including may partly reflect crop-specific differences in N use (e.g., related to C3 vs. C4 photosynthetic types), soil N pools and N dynamics (e.g.,~~ 840 ~~mineralization rates), as well as C3 vs C4 traits, soil N dynamics, weather conditions, affecting plant growth and N₂O emissions~~ but should be interpreted with caution since N supplied through mineralization of the preceding 3-year grass-clover ley is not captured in the fertilizer-N input term. So, the apparent NUE given above likely overestimates the true NUE.

The ~~substantial~~ N₂O losses ~~significantly~~ substantially affected the ~~total~~ EC-based net GHG ~~budget~~ exchange (NGHGE) of the winter wheat season, with N₂O emissions offsetting 70% of the ~~climate benefit gained from seasonal~~ net CO₂ uptake. The ~~is~~ offset ~~was~~ is considerably higher than those reported by Maier et al. (2022) for pea and maize in Switzerland (12% and 10%, respectively), ~~and it also exceeds values reported for managed Central European permanent grasslands in Central Europe, where combined N₂O and CH₄ emissions offset about 21% of CO₂ uptake (Hötnagl et al., 2018).~~ This large ~~difference is most probably related to~~ offset partly reflected the small net CO₂ sink during the winter wheat season, ~~as the ecosystem acted as a likely driven by enhanced heterotrophic respiration from decomposition of the preceding grass-clover ley residues.~~ When including lateral C fluxes, i.e., organic fertilizer inputs and harvest exports, to calculate the net ~~CO₂~~ GHG budget, winter wheat was a substantial net GHG source ~~for approximately five months, namely, consistent with net C losses and declining SOC stocks reported from long-term measurements at the same site (Emmel et al., 2018).~~ The field acted as a small net CH₄ source, consistent with results from seeding to mid March. In contrast, spring sown pea and maize did not undergo a winter phase; thus, net CO₂ release occurred only briefly during their respective cropping seasons, overcompensated by fast growth and thus high CO₂ uptake during the summer months. Since, to our knowledge, full GHG budgets for winter wheat under temperate conditions are lacking, other agricultural soils (Cowan et al., 2021). CH₄ emissions occurred mainly during wet periods, while dry periods showed low uptake, indicative of aerobic oxidation (Le Mer and Roger, 2001). The net CH₄ source likely reflected the poorly drained silty clay soil at our study ~~helps to close this gap by providing a season long, field scale budget based on continuous flux measurementssite, which likely promoted anaerobic conditions favoring methanogenesis.~~

Despite the absence of fertilizer application, the average N₂O flux during the cover crop season was only slightly lower than that ~~observed~~ during the winter wheat season (0.72 vs. 0.81 nmol m⁻² s⁻¹, respectively). This ~~unexpectedly small difference may be explained by the~~ most likely reflected low plant N uptake due to slow crop establishment ~~during the short cover crop season (60 days), resulting in low plant N uptake, while~~ and enhanced N mineralization due to warm ~~summer~~ temperatures ~~combined and post-harvest soil disturbance, as indicated by increased soil N_{min} between late May to early August (Fig. 6d).~~ Such conditions are consistent with recent ~~soil disturbance from soil preparation enhanced N mineralization of soil organic matter and residues. Recent studies have shown~~ showing that bare ~~soil conditions can or sparsely vegetated soils~~ promote N₂O ~~N₂O~~ emissions ~~due to~~ through reduced plant N uptake and enhanced microbial activity (Maier et al., 2025; Shang et al., 2024; Tallec et al., 2022; Timilsina et al., 2024), ~~which aligns well with our observations.~~ Moreover, daily mean NEE remained positive until late August (Fig. 3a), indicating that the soil ~~acted as~~ was a net CO₂ source for approximately half of the 60-day cover crop season. As a result, the cover crop season was characterized by net CO₂ release, accounting for 90% of the total GHG budget during this period ~~(Table 2), with N₂O contributing the remaining 10% was attributed to N₂O emissions, as~~ %, while CH₄ fluxes were negligible. ~~Nevertheless, the (Table 2).~~ However, this net CO₂ release reflected NEE during a short, disturbed post-harvest establishment phase rather than an intrinsic property of cover ~~crop~~ season was beneficial crops: a summer cover crop between two winter cereals is not standard practice at this site and was implemented here for the ~~overall GHG budget at the Oensingen cropland site, first time. Indeed, cover cropping reduced post-harvest GHG~~

emissions relative to bare soil: in 2019, ~~when the soil remained field was left~~ bare after the winter wheat harvest ~~until the sowing of winter barley and no cover crop was sown~~. As a result, the post harvest ~~daily post-harvest~~ CO₂-eq fluxes were approximately ~~roughly~~ double (~~16 g CO₂-eq m⁻² d⁻¹ over bare soil; Maier et al., 2025~~) compared to those measured ~~during~~ this study (~~16 vs 7.4 g CO₂-eq m⁻² d⁻¹ over cover crop~~). These elevated GHG emissions were ~~;~~ Maier et al., 2025), driven primarily ~~driven~~ by increased CO₂ emissions, ~~with N₂O contributing to a lesser extent~~. Although management and climatic conditions differed between the two years, this pronounced difference ~~in GHG budgets~~ highlights the benefit of maintaining a green cover crop ~~in summer, between two winter crops, to reduce the GHG footprint of crop production. This interpretation is also~~ consistent with ~~findings from Emmel et al. (2018), who showed through modelling that cover crops reduced CO₂ losses compared with bare soil results at the same site. These results also align with (Emmel et al., 2018) and current Swiss policy efforts promoting continuous soil cover (Art. 71c DZV, Swiss Federal Council, 2025), aimed at limiting post harvest bare soil periods and promoting continuous soil cover to reduce erosion, improve soil fertility, and nitrate losses to ground water.)~~.

4.3.4 Temporal dynamics of N₂O source processes

Stable isotope sampling on selected dates in March 2023, following fertilizations on 27-28 February, coincided with the period of highest N₂O fluxes: cumulative EC-based emissions in March alone totalled 2.5 kg N₂O-N ha⁻¹, representing 45% of total season losses over winter wheat. The FRAME model by Lewicki et al. (2022) provided a powerful framework for quantifying the relative contributions of different N₂O -producing processes over time. ~~In our study, Denitrification, in particular heterotrophic bacterial denitrification and/or nitrifier denitrification were,~~ was the dominant sources of N₂O production ~~(Fig. (Figs. 7). Interestingly, A7), consistent with poor soil drainage and persistently high WFPS (> 65% at 0.05 m), promoting anaerobic conditions which favor denitrification (Bateman and Baggs, 2005; Davidson, 1991). Improving drainage in such settings may therefore help to mitigate N₂O emissions by reducing the extent and duration of these favorable conditions for denitrification (Bouwman, 1996; Grossel et al., 2016). Nitrification and/or fungal denitrification contributed most strongly up to 22 ± 15% immediately after N-fertilization (-20%), but declined rapidly thereafter, indicating that nitrification was only a short lived contributor while denitrification remained dominant (Fig. 7). This transient response is,~~ consistent with the typical post-fertilization ~~depletion~~ of mineral N, where NH₄⁺ availability peaks and is subsequently depleted as it is oxidized to NO₃⁻ (Pérez et al., 2001). ~~At our site, the overall dominance of The near-simultaneous application of mineral N and slurry likely further promoted denitrification-related pathways likely reflects poor soil drainage (only 10% sand) and persistently high topsoil (0.05 m) WFPS levels (above 65% during the fertilization in March). Such conditions by providing both NO₃⁻ and easily degradable organic C, creating conditions favorable for heterotrophic denitrifier activity (Dittert et al., 2005). Because such high-risk combinations can create anaerobic environments that favor denitrification (Bateman and Baggs, 2005; Davidson, 1991). occur in mixed crop-livestock systems, policy and management guidance should discourage closely timed applications (Schils et al., 2008).~~

910 The initially low ~~fraction (~0.5) of~~ reduced N₂O ~~fraction (~50%)~~ following fertilization ~~might be related to~~ may reflect elevated NO₃⁻ concentrations, ~~resulting in causing~~ NO₂⁻ accumulation and inhibition of the final reduction step of N₂O to N₂ (Blackmer and Bremner, 1978; Senbayram et al., 2019). Over time, the fraction of reduced N₂O markedly increased ~~markedly~~, reaching high values on 17 March (~~~0.8; 80%~~), coincident with topsoil WFPS exceeding 80% and thus favoring complete denitrification. However, it should be noted that the isotopic signature of emitted N₂O becomes increasingly
915 uncertain at low flux magnitudes (Harris et al., 2020b). Detailed soil microbial community analyses, in combination with stable isotope analyses in N₂O, would be ~~needed~~ useful to disentangle these competing N₂O production processes, preferentially across different sites and crop rotations.

4.4 Implications for N₂O mitigation in cropland

Our findings reinforce recent studies emphasizing the critical role of vegetation as a N sink in reducing the risk of N₂O emissions from agricultural ecosystems (Feigenwinter et al., 2023; Maier et al., 2022, 2025; Tallec et al., 2022; Timilsina et al., 2024). Specifically, we identified crop establishment and early spring as two phases particularly prone to high N₂O losses during the winter wheat season. These periods were characterized by a mismatch between N supply and plant demand, driven by limited crop growth and substantial mineral N inputs from mineralization or early fertilization, resulting in surplus mineral N in the soil. This excess N, combined with favorable moisture and temperature conditions, created optimal
925 conditions for microbial N₂O production. Stable isotope data further suggested that although denitrification was the dominant process for N₂O production, high mineral N concentrations not only provided the substrates for N₂O production but may also have inhibited the complete reduction of NO₃⁻ to N₂, thereby increasing the proportion of N lost as N₂O instead of N₂ (Pan et al., 2022). To address these vulnerabilities, management strategies that promote rapid and sustained crop growth, such as optimized sowing dates and cultivar choice, are key N₂O mitigation strategies during the crop establishment
930 phase (Tallec et al., 2022; Maier et al., 2025). In early spring, mitigation will depend on better synchronizing fertilizer N inputs with crop N demand and soil N release. This can be achieved by adjusting both the timing and the amount of N application (Hoben et al., 2011; Omonode et al., 2017), including split applications, site-specific fertilization planning (Jordan Meille et al., 2023), precision fertilization (Diacono et al., 2013), and enhanced efficiency fertilizers that slow N release (Akiyama et al., 2010). Finally, site-specific soil conditions should be considered, as they can substantially influence
935 N₂O emission dynamics. At our poorly drained site, elevated soil moisture likely amplified denitrification losses by creating anaerobic conditions. Improving drainage in such settings may therefore help to mitigate N₂O emissions by reducing the extent and duration of these favorable conditions for denitrification (Bouwman, 1996; Grossel et al., 2016).

5.5 Conclusions

The XGBoost-SHAP-based approach framework proved to be an effective tool for identifying critical periods for N₂O losses
940 and not only the main drivers for each period. This provided valuable insights into the of N₂O fluxes but also their temporal

dynamicsdevelopment, allowing the identification of critical periods for N₂O emissionslosses during a winter wheat-cropping season and the subsequent summer cover crop. Thanks to its flexibility and data-driven nature, this method-couldframework can be applied to other cropping systems to improve our understanding of N₂O emission dynamics and inform targeted management. Crop establishment and early spring emerged as particularly vulnerable phases for N₂O losses, largely due to a mismatch between N supply and plant demand. This mismatch, oftenlack of synchronization, driven by slow early crop development or early fertilization, led to elevated soil mineral N levels-in the-soil, which, under favorable moisture and temperature conditions, created hotspots-hot moments for microbial N₂O production, primarily through denitrification-and/or nitrifier-denitrification-. Gross primary productivity (GPP), used here as a proxy for plantcrop activity and N uptakedemand, showed a strongconsistent negative relationship-witheffect on N₂O fluxes, emphasizing-supporting the critical role of active vegetation can play in limiting N₂O emissions. The emission factor (EF) estimated forBoth cumulative and yield-scaled N₂O emissions during the winter wheat was 1.8%, exceeding IPCC default values, and cumulative N₂O emissions were substantially higher thangrowing season exceeded those previously-reported for-in previous studies on wheat. These losses notably offset 70% of the climate benefit from net CO₂ uptake, highlighting the need for high-resolution N₂O flux measurements over-cropland-across cropland sites spanning a range of management, soil, and climate conditions, to accurately-representbetter constrain N₂O emissions in cropland GHG models-at regional and global scales-assessments. Overall, our findings underscore the importance of implementing management strategies that enhance crop growth in theidentify synchrony between N supply and plant demand, particularly during crop establishment phase-and better align N inputs-with plant N demand to reduceand early spring, as a key leverage point for reducing N₂O emissions and minimize the GHG footprint of cropwheat production.

Appendix A

Table A1. Management activities ~~conducted~~ during the 2022-2023 measurement period at the cropland in Oensingen.

Crop	Management activity	Date
Grass-clover	Harvest	20 September 2022
	Herbicide application (Glyphosate, W-5553 Sintagro)	3 October 2022
Winter wheat	Sowing (direct seeding)	6 October 2022
	Insecticide application (Sprinter, Netzmittel, Pixxarro)	12 October 2022
	Ammonium nitrate application (Mg-Ammonsalpeter, Landor)	27 February 2023
	Slurry application (dairy)	28 February 2023
	Herbicide application (Concert SX, Derux, Gondor)	22 March 2023
	Ammonium nitrate application (Mg-Ammonsalpeter, Landor)	6 April 2023
	Harvest (grain and straw)	15 July 2023
Bare soil	Soil cultivation (10 cm depth)	17 July 2023
Cover crop	Sowing	27 July 2023
	Mulching	25 September 2023
Bare soil	Soil cultivation (10 cm depth)	27 September 2023

Table A2. Summary of data gaps in EC flux time series used in this study. Gap statistics are reported for two quality-control selections: QC0, including only best-quality records, and QC0-1, including best- and medium-quality records. Gap length is expressed in time steps (1 step = 30 min), with a “gap” being a contiguous sequence of missing records. Total number of gaps, median, third quartile (i.e., 75th percentile, Q3), and maximum gap length per time series are shown. Percentage of gaps that were shorter than one day, the number of gaps longer than three days, and the number of gaps longer than one week are given as well.

Flux	QC level	# gaps	Median (steps)	Q3 (steps)	Max (steps)	% < 1 day	# > 3 days	# > 1 week
NEE	QC0	1,947	2	5	233	99.7%	1	0
NEE	QC0-1	1,782	2	4	232	99.8%	1	0
N ₂ O	QC0	2,011	2	5	459	99.5%	5	1
N ₂ O	QC0-1	2,329	1	3	441	99.6%	5	1
CH ₄	QC0	1,636	4	10	459	97.6%	6	1
CH ₄	QC0-1	2,950	2	4	458	99.7%	5	1

Table A3. Cumulative fluxes of CO₂, N₂O, and CH₄ (expressed in CO₂ equivalents) and the resulting net GHG exchange (NGHGE) for the winter wheat and cover crop seasons under three constant friction velocity (u_{*}) filtering thresholds (CUT), following Pastorello et al. (2020): the 16th percentile (CUT16), the default median threshold (CUT50), and the 84th percentile (CUT84) are given.

Period	u _* scenario	CO ₂ (g CO ₂ m ⁻²)	N ₂ O (g CO ₂ -eq m ⁻²)	CH ₄ (g CO ₂ -eq m ⁻²)	NGHGE (g CO ₂ -eq m ⁻²)
Winter wheat	CUT16	-358	232	14	-111
	CUT50 (default)	-329	237	16	-76

	CUT84	-289	243	17	-29
Cover crop	CUT16	392	46	-2	436
	CUT50 (default)	397	45	-1	441
	CUT84	418	46	-2	462

Table A4. Overview of key phenological stages of winter wheat, showing ~~the~~ observation dates and corresponding BBCH growth stage numbers during the 2022-23 growing season.

Date	BBCH
11 November 2022	13
22 December 2022	21
7 February 2023	22-23
17 March 2023	24-25
4 April 2023	31
5 May 2023	33
19 May 2023	39
31 May 2023	59
19 June 2023	73
28 June 2023	75
11 July 2023	92

990 **Table A5.** Optimized XGBoost hyperparameters for the N₂O flux driver model. Hyperparameters were selected using a randomized search with 5-fold cross-validation within the training dataset. The search evaluated 200 parameter combinations, corresponding to 1000 model fits in total. The best cross-validation RMSE was 1.85 nmol N₂O m⁻² s⁻¹.

Hyperparameter	Selected value
colsample_bytree	0.889
gamma	0.469
learning_rate	0.00508
max_depth	14
min_child_weight	5
n_estimators	260
subsample	0.722

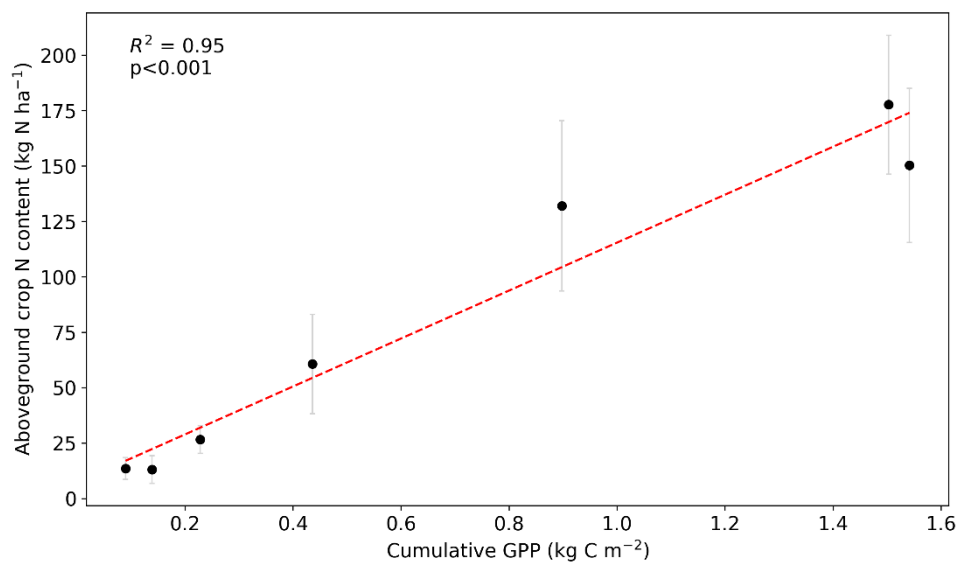
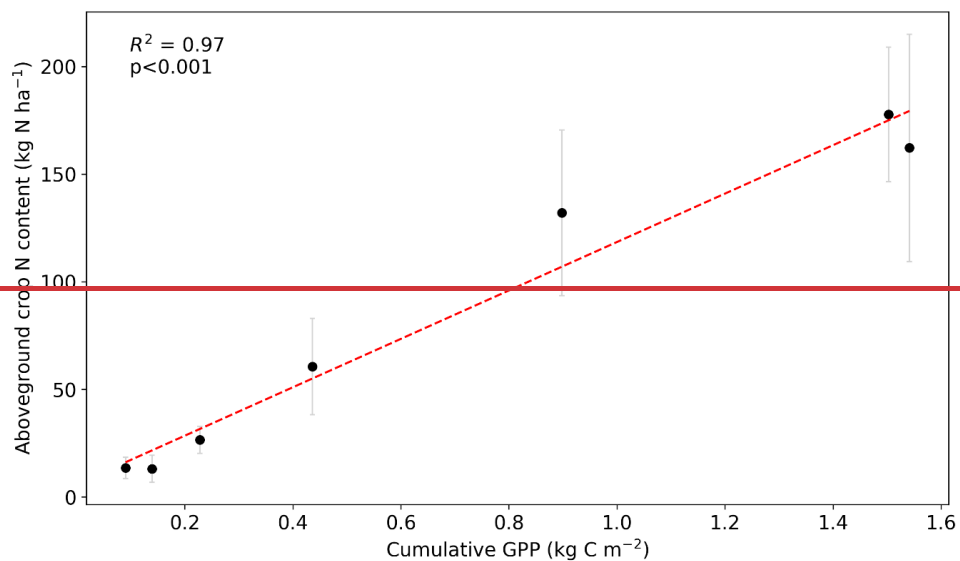


Figure A1. Relationship between cumulative gross primary productivity (GPP) and aboveground crop N content during the wheat growing season. Means $\pm$ 1 standard deviation are given (n=12). The dashed red line indicates a linear least-squares regression, with the coefficient of determination (R^2) and respective p-value shown.

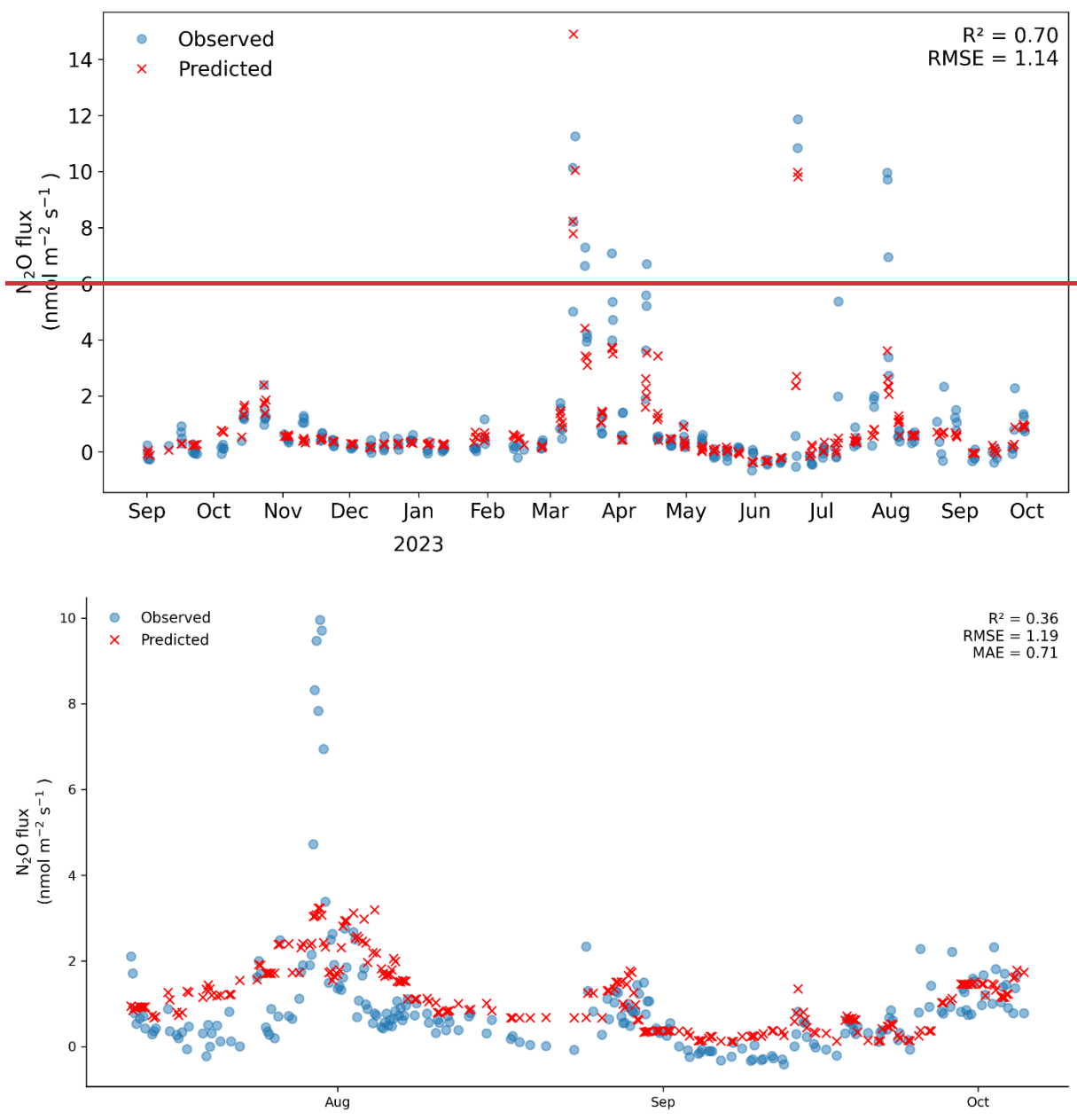


Figure A2. Observed and predicted N₂O fluxes at the cropland Oensingen for the testindependent chronological hold-out set (corresponding to the final 20% of total data)-the time series. The blue circles represent the values predicted by the XGBoost model, while the red crosses indicate the observed values. The coefficient of determination (R²) and, root mean square error (RMSE), and mean absolute error (MAE) for the testhold-out set are given.

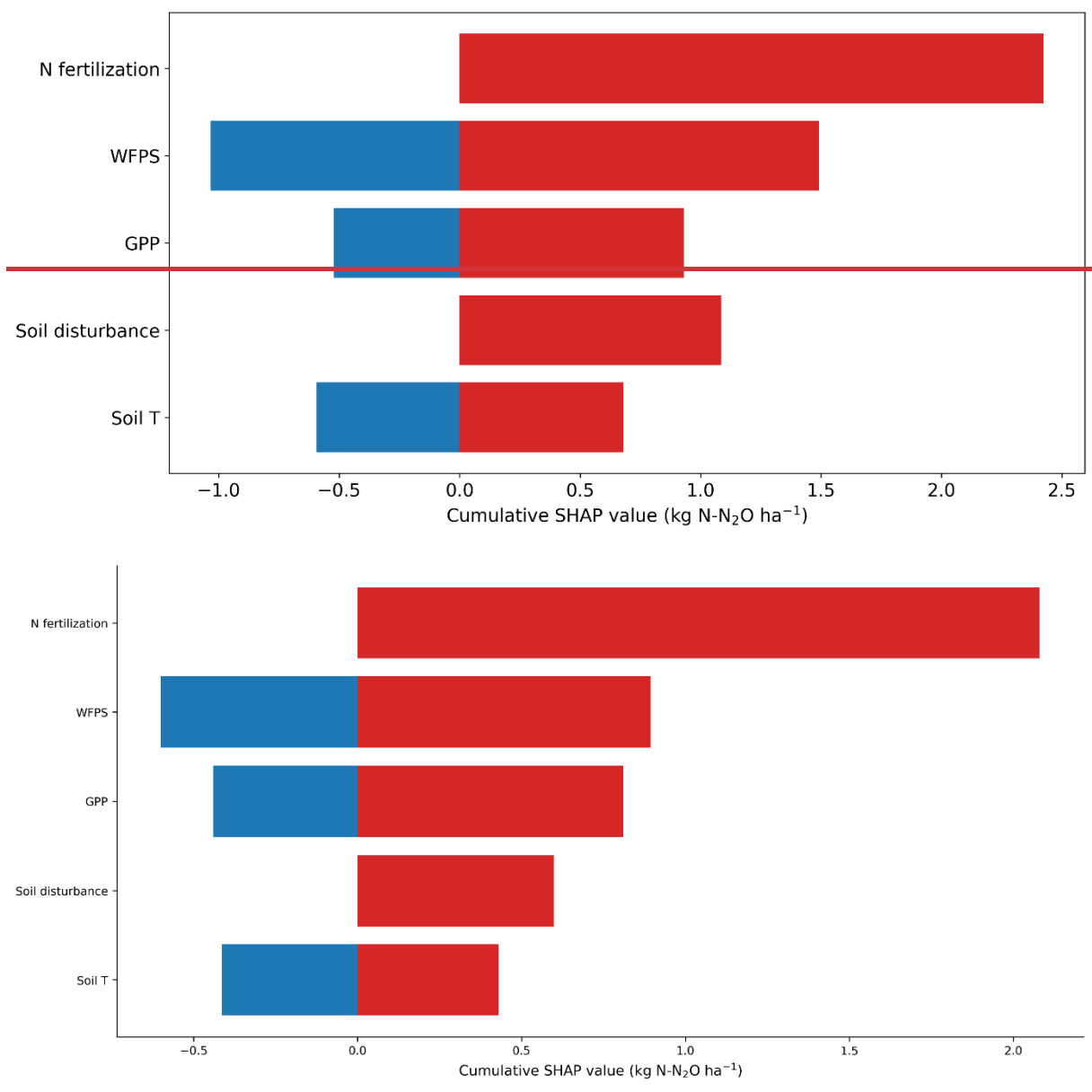


Figure A3. Cumulative positive (red) and negative (blue) SHAP contributions of each driver to predicted N₂O fluxes from September 2022 to October 2023 at the cropland Oensing. Positive and negative SHAP values were summed up separately, such that increases and decreases in N₂O fluxes are shown independently rather than cancelling each other out.

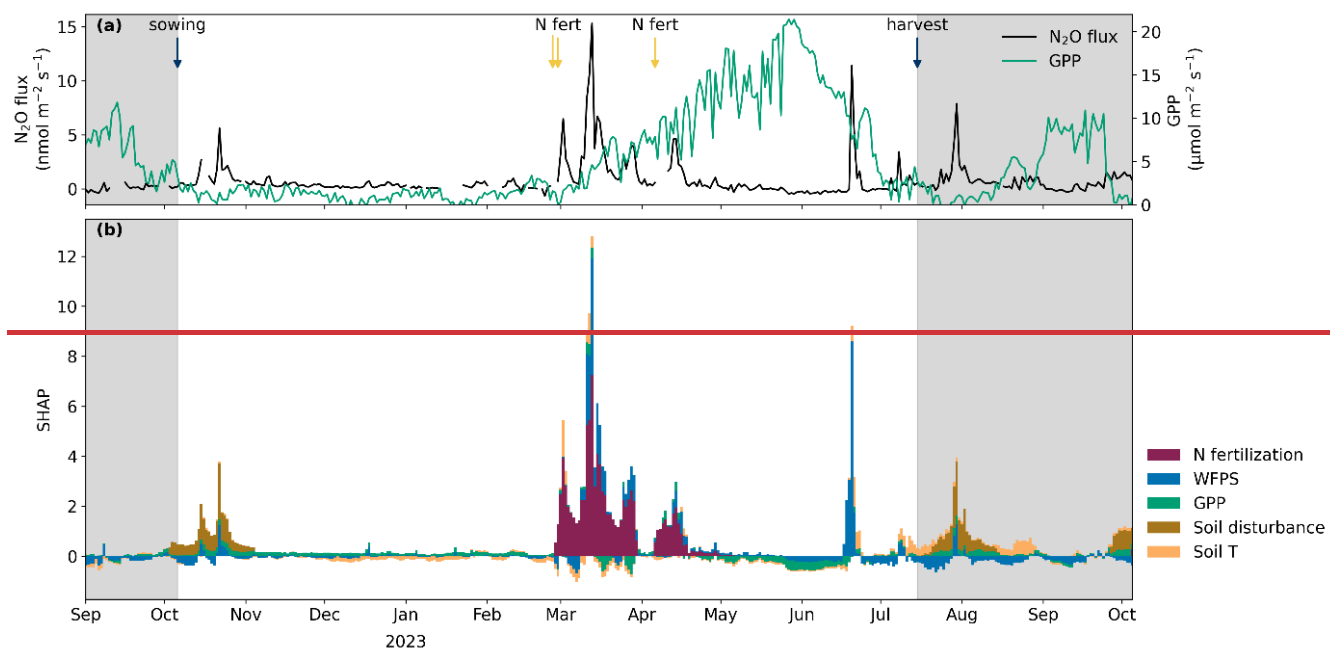


Figure A4. Temporal dynamics of N_2O fluxes, gross primary productivity (GPP), and driver contributions to N_2O fluxes at the Oensingen cropland from September 2022 to October 2023. The unshaded area corresponds to the winter wheat cropping season, while the shaded areas indicate the final phase of the preceding temporary grassland and the cover crop following winter harvest. (a) Daily average N_2O fluxes (measured, highest quality fluxes only) are shown in black, and daily average GPP in green. Arrows at the top denote management activities conducted during the winter wheat cropping season. (b) Contributions of individual drivers (i.e., N fertilization, water filled pore space (WFPS), GPP, soil disturbance, and soil temperature (soil T)) are expressed as daily averages of SHAP values (see Sect. 2.6.2 for methodological details). The baseline (SHAP = 0) corresponds to a predicted N_2O flux of $0.27\ nmol\ m^{-2}\ s^{-1}$. Positive values indicate a driver's increasing

effect on N_2O fluxes, while negative values reflect a decreasing effect.

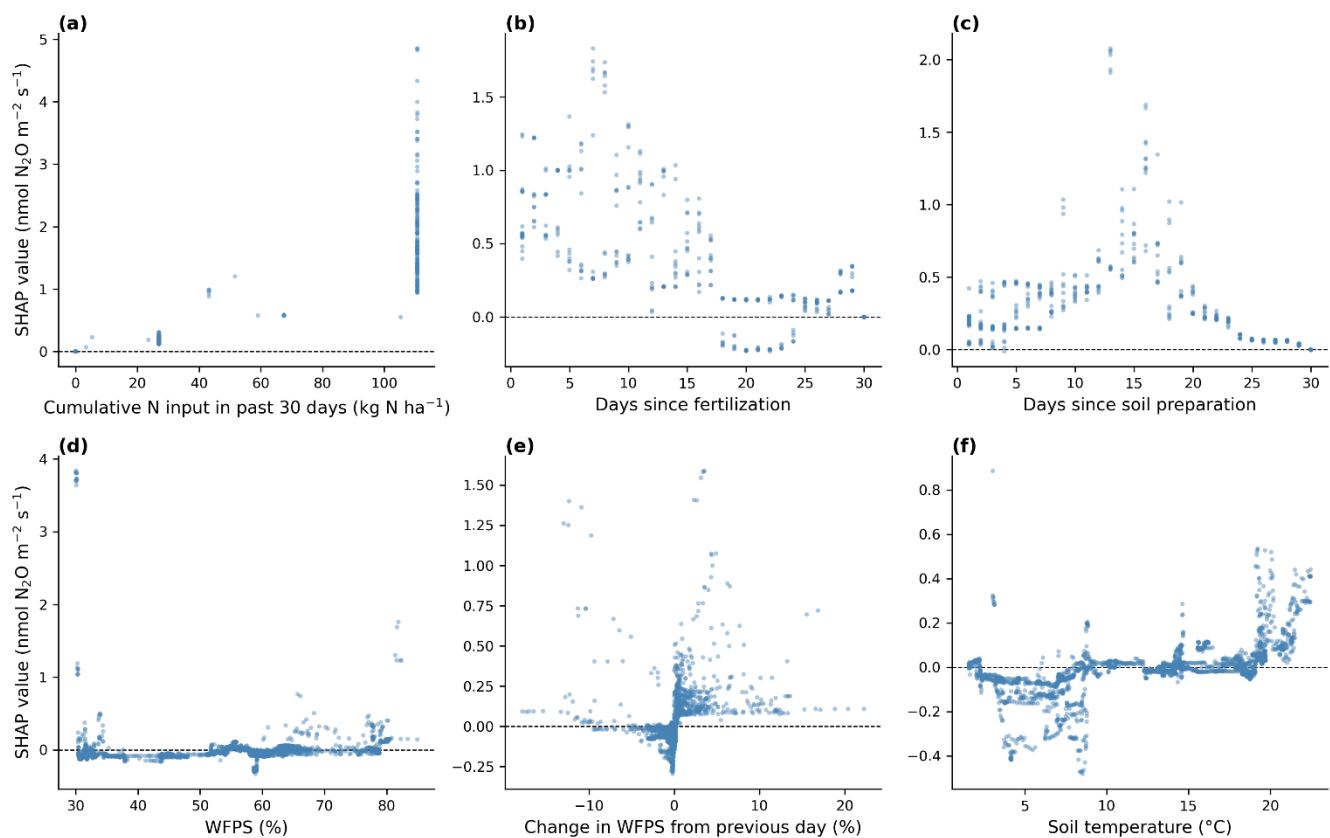


Figure A4. SHAP dependence plots for the drivers used in the XGBoost model for N_2O fluxes (except for GPP, which is shown separately in Fig. 5). Each panel shows the SHAP values of a given driver against its observed values across all data, reflecting the driver's marginal contribution to the modelled N_2O flux.

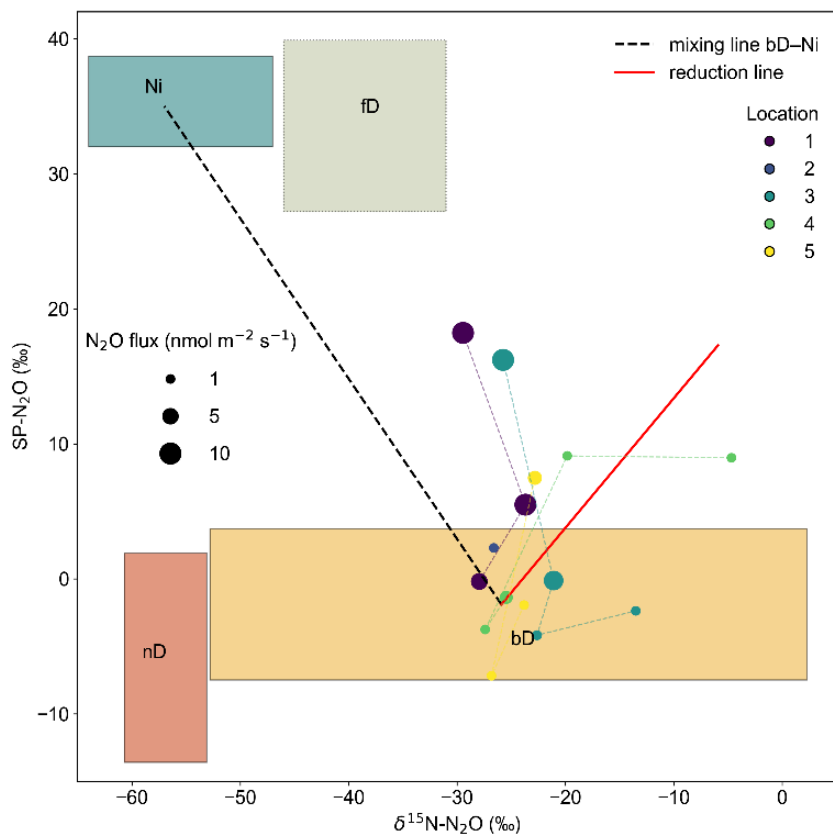


Figure A5. Dual isotope plot of $\delta^{15}\text{N}_{\text{bulk-N}_2\text{O}}$ vs. site preference (SP). Colored boxes denote N_2O mixing endmembers (nD: nitrifier denitrification, bD: heterotrophic bacterial denitrification, Ni: nitrification, fD: fungal denitrification). Endmember values are derived from (Yu et al., 2020). Lines for mixing (black) and N_2O reduction to N_2 (red) are shown. Individual measurements are shown as circles, with size reflecting flux magnitude and color indicating location (1 to 5; see Fig. 1).

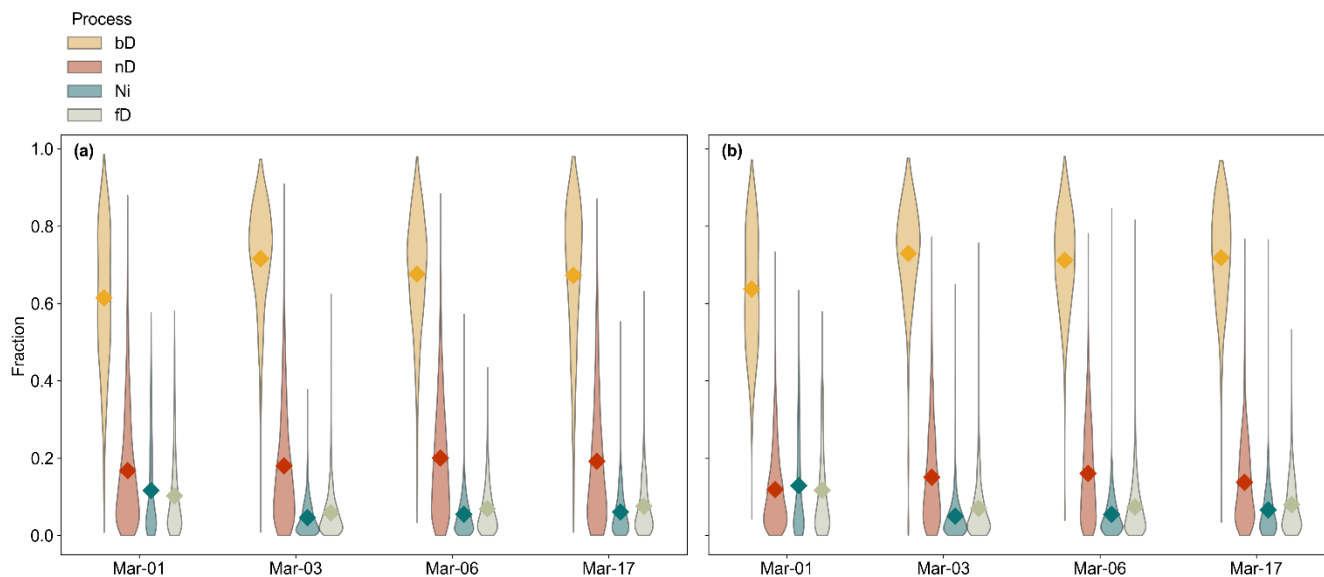


Figure A6. N_2O source fractions estimated by the FRAME model in March 2023 following fertilization (27-28 February). Two alternative model scenarios are shown: (a) mixing-reduction, and (b) reduction-mixing. Violin plots show posterior distributions for heterotrophic bacterial denitrification (bD), nitrifier denitrification (nD), nitrification (Ni), and fungal denitrification (fD). Diamonds indicate mean values.

Code availability

The Python scripts used for data analysis and visualization are available on GitHub (fabioturc/n2o-wheat-drivers-sources) and archived on Zenodo (<https://doi.org/10.5281/zenodo.1807522521222259>). Scripts used to produce the fluxes dataset are available on GitHub (fabioturc/dataset_ch-oe2_2021-23_flux_product) and Zenodo (<https://doi.org/10.5281/zenodo.17975468>).

Data availability

Eddy covariance ecosystem fluxes, meteorological data, and management information are openly available for download in the ETH Zurich Research Collection (<https://doi.org/10.3929/ethz-c-000782868>). All analysis data for this study are also openly available at Zenodo (<https://doi.org/10.5281/zenodo.1807522521222259>).

Author contributions

FT, IF, LA, FL, and NB: conceptualization of the study. FT and LH: data curation. FT: formal analysis, visualization, and writing (original draft preparation). IF, FL, and NB: supervision. FL and NB: project administration. FL and NB: funding acquisition. All authors: methodology and writing (reviewing and editing).

1050 **Competing interests**

The authors declare that they have no conflict of interest.

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