Modelling N_2O Emissions in Fertilized Grasslands with Machine Learning: A Multi-Site LSTM Approach

Samin Payrosangari[1], Kathrin Fuchs[1], Benjamin Wolf[1], Ralf Kiese[1], Clemens Scheer[1]

[1]Karlsruhe Institute of Technology, IMK-IFU, Garmisch-Partenkirchen, Germany

Correspondence to: Samin Payrosangari, Kathrin Fuchs (samin.payrosangari@kit.edu, kathrin.fuchs@kit.edu)

Abstract. Accurate quantification of GHG emissions from agricultural soils based on key environmental and management factors, is crucial for developing effective mitigation strategies. This study applies a machine learning approach using data from multiple montane grasslands in central Europe to model the spatial and temporal dynamics of N_2O emissions, using meteorological, soil, and management data. The primary aim is to advance predictive modelling of N_2O emissions from grassland soils for spatial upscaling and scenario analysis. Specifically, we assess whether a ~~generic~~regional model can accurately estimate N_2O emissions from an independent site excluded from training.

We collected data from five fertilized grasslands across southern Germany, northern Switzerland and ~~northern~~western Austria (122 soil-site-treatment-year combinations), and trained a long short-term memory (LSTM) algorithm to model the influence of drivers within 5 subsequent days on N_2O emissions. The dataset includes daily N_2O emission measurements along with key emission drivers such as soil moisture and temperature in 10 cm soil depth, daily precipitation, occurrence of fertilization events (zero or one flag), as well as soil characteristics such as pH and bulk density.

~~The trained LSTM model showed strong predictive performance (RMSE of 18 $\mu gm^{-2}h^{-1}$, and Relative RMSE of 270%) when evaluated on a test set that included both data from an independent soil and withheld years from training procedures.~~

The trained LSTM model showed promising predictive performance when evaluated on two test datasets. One test set included temporally independent data (hold-out years) (RMSE = 27 µg N_2O-N m^{-2} h^{-1}), while the other included cross-site data from a soil type withheld from training (RMSE = 10 µg N_2O-N m^{-2} h^{-1}). The model captured N_2O dynamics, including the magnitude and timing of emission peaks driven by slurry application and environmental factors in many cases, while it shows error in some other cases. These results demonstrate that LSTM-based models can reliably predict N_2O emissions for most site-years across test sites with similar environmental and soil characteristics and represent a promising alternative to process-based models for predicting soil N_2O emissions.

1 Introduction

Greenhouse gas (GHG) emissions significantly contribute to global warming, with agricultural activities accounting for approximately 12% of global anthropogenic GHG emissions (Chataut et al., 2023). The greenhouse gases emitted from soils are mainly methane (CH_4), nitrous oxide (N_2O) and carbon dioxide (CO_2), which are increasing due to high-energy-intensive agricultural production systems and the production and use of mineral and organic fertilizers (Chataut et al., 2023). Today, agricultural activities are responsible for approx. two-thirds of total anthropogenic N_2O emissions and its high global warming potential makes it the third-most important anthropogenic greenhouse gas for global warming (Schulz et al.,2021; Fuchs et al., 2020). Thus, agricultural mitigation strategies play an important role in reducing N_2O emissions, which requires understanding the effects of management adoption (Fuchs et al., 2018).

The production of N_2O in the soil is driven by microbial processes — predominately denitrification and nitrification — which are influenced by both environmental conditions and management practices (Wang et al., 2021; Butterbach-Bahl et al., 2013). Key soil and environmental conditions regulating these processes include soil moisture, temperature, texture, nitrogen content, pH, and organic matter content, while fertilization, tillage, and irrigation represent the most important management practices (Wang et al., 2021; Butterbach-Bahl et al., 2013). The correlation between daily N_2O emissions and individual input drivers might be low and it's the interaction of drivers such as precipitation and temperature, as well as management practices that result in highly dynamic, variable and site-specific emission patterns (Wang et al., 2021). Thus, the complex influences of different drivers on emissions need to be simulated via high-performance models. This is especially relevant as direct measurement over large areas and long time periods is impractical (Butterbach-Bahl et al., 2013; Giltrap et al., 2010).

Modelling approaches for estimating N_2O emissions from agricultural systems include emission factors, statistical models, and process-based models (Butterbach-Bahl et al., 2013). Emission factors, i.e., a fixed proportion of applied nitrogen that is emitted as N_2O, are widely used for national inventory reporting. However, they are unable to reflect the variability of soil and climate conditions that are relevant for N_2O emissions at the field scale or with a time resolution higher than yearly (Giltrap et al., 2010). In contrast, process-based models such as LandscapeDNDC (Haas et al., 2013) or Daycent (Parton et al., 1998) simulate the interactions between soil processes, climatic drivers and management. To this end, these models use a large set of parameters, which need to be parameterized based on calibration and validation datasets. As a consequence, uncertainty of model results due to parameterization is inevitable and the performance of such models heavily depends on the number and quality of calibration and validation datasets.

Given these limitations, machine learning (ML) offers a promising alternative or complementary approach to process-based modelling. ML models are trained on previous measurements and do not require a deep understanding or a definition of the underlying processes and parameters. However, implementing a high-accuracy ML model comes with challenges, such as the need for large, high-quality datasets and expert knowledge about the used algorithms, along with lower interpretability than process-based models. While implementing the right ML model requires effort, once a generalized model is built, applying it to new data is highly time-efficient.

Building an ML model for estimating N_2O emissions requires considering short-term fluctuations and peaks in N_2O emissions in response to temporal dynamics in soil moisture and temperature, such as dry–wet transitions, water logging, as well as management activities (Butterbach-Bahl et al., 2013). Therefore, estimating daily values of N_2O emissions can be improved by considering the changes in drivers over several days prior to the emission event, which is addressed in this study. Long short-term memory network or LSTM (Hochreiter and Schmidhuber, 1997) is a machine learning model that detects the dynamic relationships in sequential data. It has previously been used for different applications such as flood forecasting (Le et al., 2019), stock market prediction (Chhajer et al., 2022), and predicting water table depth in agricultural areas (Zhang et al., 2018), and therefore is a promising method for modelling soil N_2O emissions.

In this study, we developed an LSTM model to simulate the daily N_2O emissions of grasslands in central Europe, with the three main objectives:

1) to train an LSTM model using data from multiple soils and climates to simulate daily N_2O emissions at alpine grasslands
2) to test the model performance on an independent grassland soil not used for model training to assess the ~~general~~regional applicability of the model to pre-alpine grasslands without site-specific parametrization
3) to assess the relative importance of different environmental and management variables for predicting N_2O emissions

2 Materials and methods

Daily and growing season N_2O emission data were collected from multiyear field experiments of 5 grassland sites representing a variety of soils at different elevations and thus climate conditions in Central Europe: South Germany (Fendt, Rottenbuch and Graswang), ~~north~~west Austria (Neustift) and North Switzerland (Chamau). Table 1 shows the characteristics of these grasslands, all of which are managed with organic fertilizer (manure and slurry) and cutting. While N_2O emissions were highest at Chamau, lowest N_2O emissions were observed at the Neustift site. The collected dataset for training the LSTM model includes daily measurements of soil N_2O emissions, soil physical and chemical properties (Table 2), as well as daily meteorology. The amount of daily fluxes always expresses N_2O-N amount in this paper.

Grassland	Elevation (m a.s.l.)	Annual N_2O-N (kg ha^{-1} y^{-1})	Annual precipitation (mm)	Avg annual air temperature (°C)	pH	BD (g cm^{-3})
Chamau Switzerland (CH-Cha)	393	5.28	1179	9.8	6.5	0.94
Fendt Germany (DE-Fen)	595	2.83	962	9.3	4.8-6.5	0.8-1.1
Rottenbuch Germany (DE-RbW)	769	1.69	1047	8.6	4.8-5.7	0.7-0.95
Graswang Germany (DE-Gwg)	864	2.55	1464	7	5.1-6-6	0.52-0.78
Neustift Austria (AT-Neu)	970	0.03	852	6.5	5.7	1.2

Table 1 Summary of the properties of grasslands in different climates and elevation used in this study (Kiese et al., 2018; Soltani et al., 2018; Gilgen & Buchmann, 2009; Roth, 2006; Hörtnagl et al., 2014). The total annual N_2O-N is averaged over different years of data availability for each grassland.

2.1 Site descriptions

German Terrestrial Environmental Observatories (TERENO) Pre-Alpine

The Tereno Pre-Alpine observatory includes three grassland sites, Graswang (DE-Gwg), Rottenbuch (DE-RbW), and Fendt (DE-Fen), at elevations of 864, 769, and 595 m a.s.l. respectively, which are located in the Bavarian Prealps in southern Germany (Kiese et al., 2018; Soltani et al., 2018). Automatic chamber measurements of N_2O emission along with a wide range of other measurements such as soil moisture and temperature are conducted by the Karlsruhe Institute of Technology (KIT). The automatic chamber measurements are carried out on 36 lysimeters, i.e., soil cores with 1.0 m^2 surface and a depth of 1.4 m (Kiese et al., 2018). A subset of 18 out of 36 soil cores are translocated from the high-elevation site Graswang and the medium-elevation site Rottenbuch to the lower altitude sites (space-for-time-approach), referred to as Graswang in Fendt, Graswang in Rottenbuch or Rottenbuch in Fendt translocations to investigate the soils under climate change scenarios (Kiese et al., 2018). The lysimeter setup for these grasslands is shown in Fig. A1 of appendix A. Experiments on each lysimeter follow intensive or extensive management treatments, where extensive management includes up to three cuts and two manure applications, and intensive management includes up to six cuts and five slurry applications per year (Kiese et al., 2018). From each soil and treatment three replicates are considered, for instance, there are three Graswang in Fendt soil core replicates which are intensively managed as shown in Fig. A1. Notably, at the time of this study, sub-daily (up to 6 flux rates per day) data from 24 lysimeters operated in Fendt (Fig. A1 a) and Graswang (Fig. A1 c), which are aggregated (averaged) into daily are used according to availability of data for different years between 2014 and 2020. The soil properties of different replicates (N=3: L1-L3) are shown in Table 2.

Switzerland FLUXNET Chamau

Chamau (CH-CHA) is a permanent grassland site that was established by ETH Zurich in 2005 (Feigenwinter et al., 2023) and is part of Swiss FluxNet initiative. This site is located in the Reuss River valley on the Swiss Plateau, approximately 30 km south of the city of Zurich, Switzerland, at an elevation of 393 m a.s.l. Half-hourly eddy-covariance measurements of N_2O and CH_4 started at this site in 2012 (Merbold et al., 2014). Moreover, a N_2O mitigation experiment, from 2015 to 2020, was conducted by establishing separate parcels in the northern and southern parts of the site, continuing slurry fertilization on the control parcel in the south and oversowing the north parcel with a clover seed mixture without fertilization (Fuchs et al., 2018). The non-gap-filled measurements from the control parcel aggregated (averaged) into daily values are used in this study, which represent an intensively managed site with cutting 4–5 times a year followed by liquid slurry application plus one slurry application in spring each year (Feigenwinter et al., 2023; Hörtnagl et al., 2025; Fuchs et al., 2018).

Austria Neustift

The Neustift grassland (AT-NEU) is an intensively managed meadow in the middle of a flat valley at the bottom of the Stubai valley in the Austrian alps, at an elevation of 970 m a.s.l (Hörtnagl & Wohlfahrt, 2014). The N_2O and CH_4 emissions at this site were measured between April 2010 and February 2012, and the management consisted of three cuts and one solid manure and slurry application in autumn each year, which was considered an intensively managed site (Hörtnagl & Wohlfahrt, 2014; Hörtnagl et al., 2018). At this site, fluxes were calculated via virtual disjunct eddy-covariance, providing half-hourly gap-filled flux measurements by Hörtnagl & Wohlfahrt (2014), which we ~~aggregated~~averaged to daily values for this study.

Soil	Climate (Grassland)	Replicate-Management	Clay 0-10 cm (%)	Silt 0-10 cm(%)	Sand 0-10 cm (%)	SOC 0_10 cm (%)	Nt 0_10 cm (%)	C/N 0_10 cm	pH 0_10 cm	Bulk density 0_10 cm (gr cm^{-3})	Dataset assignment	Data availability years	Dataset size
Graswang	Graswang	L1-Intensive	55	42	3	11.4	1.2	9.48	6.40	0.52	Train	2020	277
Graswang		L2-Intensive	38	43	19	8.7	0.81	10.74	5.43	0.73	Train	2020	273
Graswang		L3-Intensive	59	35	6	7.9	0.83	9.53	6.02	0.68	Train	2020	269
Graswang		L1-Extensive	60	35	5	8.5	0.87	9.72	6.07	0.65	Train	2020	284
Graswang		L2-Extensive	58	39 0	3	11.1	1.13	9.86	6.45	0.55	Train	2020	284
Graswang		L3-Extensive	37	44	19	8.1	0.75	10.80	5.20	0.80	Train	2020	283
Graswang	Fendt	L1-Intensive	61	36	3	10.9	1.15	9.43	6.56	0.55	Train/Temporal test	2014-2019/2020	744/172
Graswang		L2-Intensive	37	44	19	7.5	0.73	10.27	5.35	0.78	Train/Temporal test	2014-2019/2020	979/224
Graswang		L3-Intensive	61	35	4	8.5	0.9	9.44	6.12	0.66	Train/Temporal test	2014-2019/2020	1005/258
Graswang		L1-Extensive	57	40	3	11.3	1.195	9.42	6.40	0.52	Train/Temporal test	2014-2019/2020	1076/245
Graswang		L2-Extensive	58	38	5	7.7	0.81	9.51	6.12	0.53	Train/Temporal test	2014-2019/2020	915/238
Graswang		L3-Extensive	38	43	20	8.0	0.82	9.76	5.10	0.77	Train/Temporal test	2014-2019/2020	1039/213
Fendt		L1-Intensive	25	40	35	5.2	0.52	9.92	5.87	0.93	Train/Temporal test	2014-2019/2020	915/228
Fendt		L2-Intensive	30	43	27	4.5	0.45	9.89	4.87	1.01	Train/Temporal test	2014-2019/2020	876/260
Fendt		L3-Intensive	33	46	21	6.4	0.68	9.35	5.16	0.78	Train/Temporal test	2014-2019/2020	1095/252
Fendt		L1-Extensive(2014-2018), Intensive(2019-2020)	27	42	30	5.5	0.57	9.72	5.72	0.86	Train/Temporal test	2014-2019/2020	1012/240
Fendt		L2-Extensive(2014-2018), Intensive(2019-2020)	31	42	28	4.4	0.45	9.69	4.90	0.96	Train/Temporal test	2014-2019/2020	714/258
Fendt		L3-Extensive(2014-2018), Intensive(2019-2020)	34	45	21	6.4	0.69	9.32	5.26	0.81	Train/Temporal test	2014-2019/2020	751/255
Chamau	Chamau	Intensive	19	45	36	3.2	0.33	9.79	6.50	0.94	Train/Temporal test	2013, 2014, 2016, 2019,2020/ 2015	1420/ 320
Neustift	Neustift	Intensive	4	43	53	3.0	0.28	10.71	5.70	1.20	Train	2010-2011	259
Rottenbuch	Fendt	L1-Extensive(2014-2018), Intensive(2019-2020)	40	41	19	7.0	0.725	9.66	5.73	0.69	Cross-site Test	2014-2020	1320
Rottenbuch		L2-Extensive(2014-2018), Intensive(2019-2020)	24	42	34	4.3	0.44	9.75	5.34	0.95	Cross-site Test	2014-2020	1452
Rottenbuch		L3-Extensive(2014-2018), Intensive(2019-2020)	23	53	24	5.8	0.63	9.19	5.43	0.81	Cross-site Test	2014-2020	1478
Rottenbuch		L1-Intensive	24	43	33	4.4	0.47	9.32	4.84	0.93	Cross-site Test	2014-2020	1554
Rottenbuch		L2-Intensive	36	40	24	6.2	0.63	9.84	5.39	0.70	Cross-site Test	2014-2020	1532
Rottenbuch		L3-Intensive	28	49	23	5.9	0.65	9.08	5.18	0.80	Cross-site Test	2014-2020	1354

Table 2 Soil properties of the different soils in various climates used in this study (Kiese et al., 2018; Soltani et al., 2018; Gilgen & Buchmann, 2009; Roth, 2006; Hörtnagl et al., 2014). All soil properties refer to measurements in 0-10 cm depth. Dataset size refers to the number of daily flux observations.

2.2 Input variables and model setup

In this study we model the average daily N_2O-N emissions based on the temporal and static drivers available in the collected dataset. The temporal drivers used by the model are the daily averages of soil moisture and temperature at 10 cm soil depth, total precipitation, and the occurrence of a fertilization event. The model also incorporates static inputs, such as soil pH and bulk density, to represent the soil's chemical and physical properties across the different sites. ~~Each individual data point of the problem can be expressed as Eq. 1:~~To estimate the daily N_2O-N emission, the sequential LSTM model walks through the data sequences and in each round processes a subsequence of length 5 which include the information as Eq. 1 for estimating average daily fluxes:

$$\begin{Bmatrix} Soil\ mois_{t-4} & Soil\ temp_{t-4} & Precipitation_{t-4} & Fertilization_{t-4} \\ Soil\ mois_{t-3} & Soil\ temp_{t-3} & Precipitation_{t-3} & Fertilization_{t-3} \\ Soil\ mois_{t-2} & Soil\ temp_{t-2} & Precipitation_{t-2} & Fertilization_{t-2} \\ Soil\ mois_{t-1} & Soil\ temp_{t-1} & Precipitation_{t-1} & Fertilization_{t-1} \\ Soil\ mois_{t} & Soil\ temp_{t} & Precipitation_{t} & Fertilization_{t} \end{Bmatrix}, \{pH, BD\} \longrightarrow \{N_2O - N_t\} \quad (1)$$

Temporal Static Target

The indices indicate the values of the features at different days in which day t is the current day. The average daily N_2O-N emissions at day t is the target of the machine learning model.

The implemented sequential LSTM models in this study rely solely on the temporal and static input features shown in Eq. 1 in both training and testing phases, and no information from the N_2O-N emissions on previous days is used for learning the N_2O-N emission of the current day.

2.3 Dataset structure and pre-processing

The availability of a diverse dataset that includes translocated soil cores across German grasslands, also using data from Switzerland and Austria gives this study the opportunity to cover a variety of soils in different climates (Table 2), which is key in creating a regional model capable of transferring results across sites.

At German sites, replicates sampled from individual grassland often exhibit varying soil properties, as they are taken from different sections of expansive grassland areas. Therefore, for training the model the data from each replicated lysimeter was used separately so that the model could learn the role of soil properties in more detail.

~~Splitting the dataset to training and test sets is not done by random shuffling, but according to the objective of the study a different approach is taken. We split the dataset based on year and management technique and completely exclude the Rottenbuch soils from the model development process to consider it as an independent soil to assess the transferability of the model. For the training set, the following prerequisites are considered: 1) include treatments with a variety of soil properties, N_2O emission patterns and climates; 2) include soils with intensive treatment to ensure that the model has enough data points with fertilization events to learn the role of fertilizer under different conditions; and 3) the data from Neustift was only used for training, as a grassland with highest altitude and lowest emissions. The training set includes around 13000 data sequences in total.~~

~~On the other hand, for the test set, 3 important criteria are considered according to the goals of the study: 1) Firstly, from the Chamau soil some years are used for training, and 1 year data used as a test set to show the ability of the model in gap-filling this site for unseen years; 2) secondly, from Fendt and Graswang soils, some of the lysimeters with extensive management are used for testing, 3) Finally, all the available data from the Rottenbuch site is held back for use as an independent test soil. The test set includes around 15000 data sequence.~~

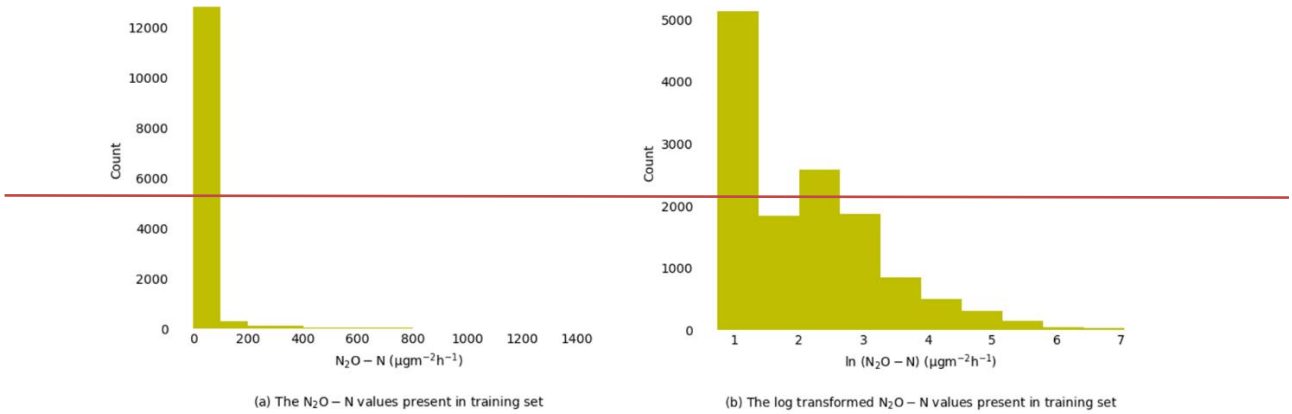
We split the dataset based on temporal hold-out as well as cross-site approaches to assess the transferability of the model in temporal and spatial scale. The training set includes treatments with a variety of soil properties, N_2O emission patterns and climates which includes (1) several years from Chamau, Fendt and Graswang soils with intensive and extensive treatments and (2) the full dataset from the Neustift site due to its limited sample size. Neustift represents the highest-altitude grassland with the lowest emissions and therefore provides important information for training the model. The training set includes around 14500 data rows in total. During the training process, the training dataset partitions into training and validation parts following a random 80:20 split as a requirement for machine learning model training. The training partition is used to fit the model, while the validation partition facilitates hyperparameter optimization—such as learning rate decay—and helps monitoring model's progress during training.

On the other hand, the test set which was completely unseen during the training, was chosen according to the study's objectives:1) Temporal test set: One year of data from Chamau, and all treatments of Fendt and Grasswang soils is held back from the training to be used as a test set. This demonstrates the model's ability to predict data from unseen years, which is consistent with the temporal training/testing split used for time series forecasting. This test set includes 3,160 data rows, (2) cross-site test set: This test set is for spatial evaluation and utilises all available Rottenbuch soil data. The cross-site test set encompasses approximately 8,690 data rows.

Along with properly splitting the dataset, data cleansing and pre-processing is crucial for training the ML model. In this study the quality checked measured data from which the gaps were excluded are used. In addition, scaling the data prior to training ensures faster convergence and improves model performance by preventing features with larger magnitudes from disproportionately influencing the learning process. The input drivers are all scaled via the Scikit-learn library robust scaler (Pedregosa et al., 2011) shown in Eq. 1. The choice of using robust scaler is made after investigating other options such as standardization and normalization (min–max scaler) for all or individual drivers according to their distribution. The robust scaler transforms each feature by removing the median and scaling it according to the interquartile range, making it robust to outliers. For each variable x, the scaled value x_{scaled} is computed via Eq. 2:

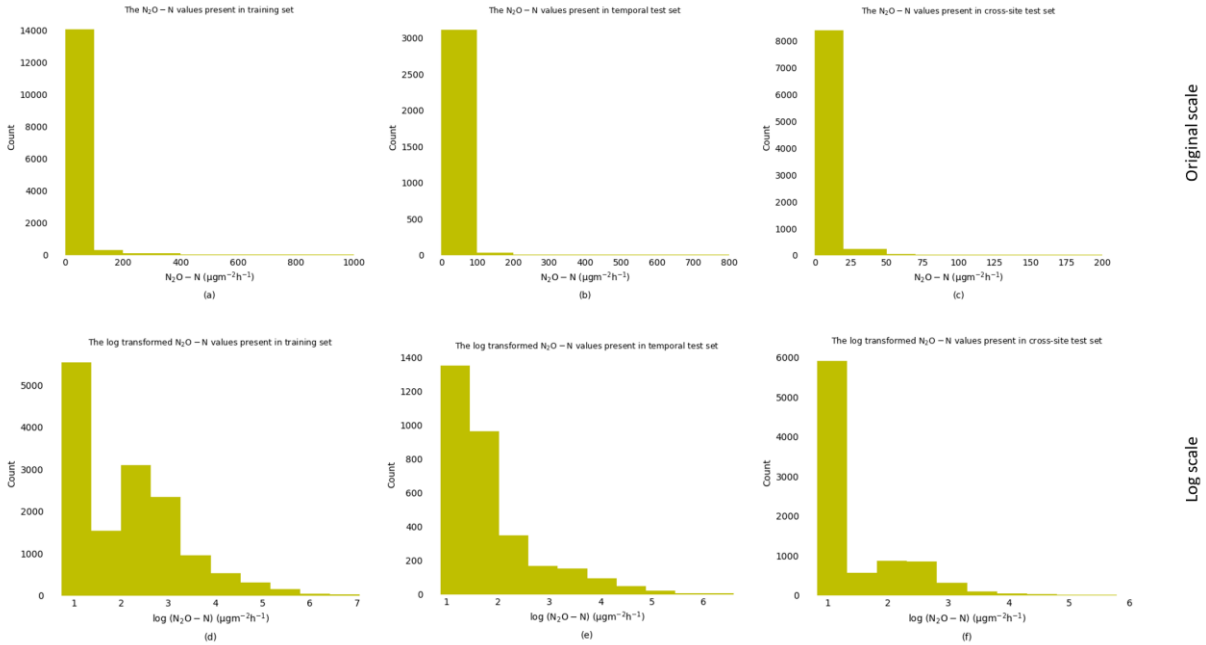
$$x_{scaled} = \frac{x - Median(x)}{Q_3(x) - Q_1(x)} \quad (2)$$

Moreover, the target value (daily N_2O-N emission) is log-transformed via natural logarithm (ln) for model setup, as its original values show a highly right-skewed distribution as shown in Fig. 1. Therefore, the output of the model is generated at log-scale and subsequently needs to be back transformed to the actual emission scale via the exponential function. Logarithmic transformations are widely used to reduce skewness and stabilize variance in heteroscedastic data (West, 2021; Hastie et al., 2009; Box & Cox, 1964). Large differences in gradient magnitude and high stochastic gradient variance are known to impair optimization and cause slow convergence in deep neural networks (Goodfellow et al., 2016); hence, variance-stabilizing transformations can yield better-conditioned gradients, more stable training and faster convergence (Salinas et al., 2020; Smyl, 2020).



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~~Figure 1 Histogram of (a) original and (b) log-transformed daily N_2O-N emissions values at the training set used in this study. Max N_2O emission value equals to 1155 $\mu gm^{-2}h^{-1}$, min value equals to 0.09 $\mu gm^{-2}h^{-1}$ and average equals to 17.5 $\mu gm^{-2}h^{-1}$ among the 13000 training datapoints.~~



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Figure 1 Histogram of original and log-transformed daily N_2O-N emissions values in the dataset used in this study. Panels a-c show the original values, and panels d-f show the log-transformed (natural log) values for the training set, temporal test set and cross-site test sets respectively.

2.4 Model development and training procedure

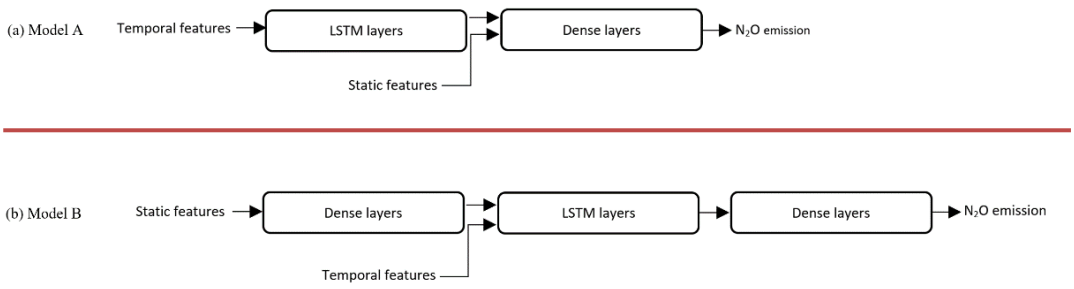
To build a model based on LSTM neural networks with high performance in simulating daily N_2O-N emissions, different aspects such as the architecture of the neural network, scaling and transforming the data, selecting a proper loss function for training and hyperparameter tuning were considered. In this section, the methods used in this study for model development are explained.

2.4.1 LSTM model architecture

Long short-term memory (LSTM) is a type of recurrent neural networks (RNN) that learns long-term dependencies in sequential data and is often used in speech recognition and time series processing (Hochreiter and Schmidhuber, 1997). As discussed in previous sections, simulation of daily N_2O-N emissions from soil is more accurate if the role and changes in environmental conditions over several days are simulated using a sequential model. In this study, we built the LSTM network architecture as shown in Fig. 2, which was implemented using the Keras library in Python (Chollet et al., 2015). The model architecture is investigated with various configurations and hyperparameters to find the optimum model.

~~The first architecture, Model A, firstly processed the temporal inputs (Eq. 1) via a set of LSTM layers. Subsequently, several dense layers that receive the output of the LSTM layers as well as a set of static inputs (pH and bulk density) are added to be processed by the model.~~

~~In contrast, the second architecture, Model B, initially processes the static inputs via dense layers, then uses the processed information as an initial input to a set of LSTM layer (initializing the hidden state of first LSTM layer) and includes the temporal inputs at this stage.~~



~~Figure 2 Two basic architectures of the LSTM tested in this study.~~

The model in this study initially processes the temporal inputs (Eq. 1) via 3 LSTM layers. Subsequently, an attention layer processes the output sequence of the last LSTM layer. Afterwards, the set of static inputs (pH and bulk density) are concatenated to the output of previous layers to be processed by the model. Figure 2 shows the model's architecture. The models in this study are built with an attention mechanism. Attention in LSTM refers to a mechanism that allows the model to dynamically focus on specific parts of the input sequence when generating each output, improving performance by weighting relevant hidden states (Bahdanau et al., 2015).

In problems with both temporal and static features, there is an alternative possible architecture which initially processes the static inputs via dense layers, then uses the processed information as an initial input to LSTM layers (initializing the hidden state of first LSTM layer). However, since this alternative architecture showed low performance for our dataset we did not further investigate it.

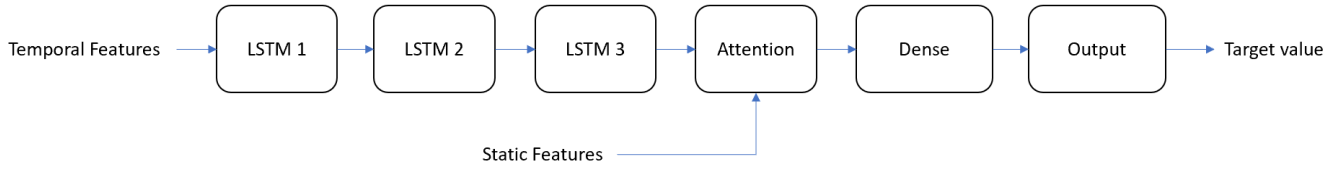


Figure 2 Architecture of the LSTM model used in this study. The LSTM implementations is available in the repository provided in Data and code availability section.

2.4.2 Loss function

The loss function used during training quantifies the error between the model's predictions and the actual target values, guiding the optimization process to minimize this error. For the current imbalanced dataset, a custom loss function is used to highlight the importance of catching high peaks of N_2O-N emissions which is formulated in Eqs. (3) and (4) as:

$$loss = abs(y_{true} - y_{pred}), \quad (3)$$

$$weighted\ loss\ = loss * e^{loss_coefficient * loss}, \quad (4)$$

With y_{true} and y_{pred} representing the observed and predicted daily N_2O-N fluxes, respectively. This loss function is significantly penalizing the model for high errors in peak values and showed a better performance comparing to the mean squared error (MSE), mean absolute error (MAE) as well as weighted mean squared (WMSE) error. In addition, loss_coefficient is a hyperparameter controlling the exponential weight further, with potential values shown in Table 3.

2.4.3 Hyperparameter tuning

Hyperparameter tuning is a key step in developing machine learning models, as it helps identifying the best-performing configuration for a given problem. Hyperparameters influence the model's complexity, learning ability, and performance. The main hyperparameters used in this study and their tested ranges are shown in Table 3. In this study, Hyperband algorithm (Li et al., 2018) was used at initial stages to optimize the hyperparameters of the LSTM model, followed by manual adjustments based on dataset characteristics to improve the model's ability in capturing fluctuations and rare high peaks more accurately.

Hyperparameter	Value ranges
Learning rate	[1e-2, 1e-3]
Activation functions for dense layers	[Tanh, Relu, Leaky relu, Linear]
Activation functions for LSTM layers	[Tanh, Relu]
Number of neurons	20-65
LSTM layers recurrent L2 regularization	[1e-4,1e-3,1e-2]
LSTM layers kernel L2 regularization	[1e-4,1e-3,1e-2]
Dense layers L2 regularization	[1e-4,1e-3,1e-2,1e-1]
Dropout	[0.01,0.05,0.1, 0.2,0.5]
Number of LSTM Layers	3-5
Number of dense layers	2-3
loss_coefficient used in the loss function	[1,1.2, 1.5]

Table 3 Ranges of hyperparameters of the model considered for hyperparameter tuning in this study. The best hyperparameters are available in the repository provided in Data and code availability section.

2.4.4 Feature importance in LSTM

This study applies the permutation feature importance (PFI) method introduced by Breiman (2001), which calculates the contribution of each feature to the model's estimation of N_2O-N emissions. This technique shuffles the value of an individual feature in the dataset, calls the model and observes the degradation of the model performance, which is now producing results with this feature having shuffled values (Breiman, 2001). Therefore, we define the relative importance metric of each feature as the degree of increase in the mean squared error (MSE) in comparison to the MSE in the original model, formulated in Eq. 5:

$$\textit{Relative importance feature } m = \textit{MSE PFI feature } m - \textit{MSE original model} \quad (5)$$

2.6. Post-processing and statistical analysis

~~To assess model performance, we used the RMSE and relative RMSE, which is defined as the RMSE divided by the mean value of the target variable in percentage. In addition, for the analysis of the results time series plots for daily emissions as well as cumulative plots for yearly cumulative emissions are created in Matplotlib, Python (Hunter 2007).~~

We report the coefficient of determination R^2 (Montgomery et al., 2021), the mean absolute error MAE and root mean squared error RMSE (Willmott & Matsuura, 2005), as well as bias (mean difference between modelled and observed values) to indicate the model's performance. In addition, we report Spearman's rank correlation coefficient ρ and its 95% confidence interval (Spearman, 1904; Bonett and Wright, 2000) to capture monotonic relationship between modelled and observed values. Several metrics for interpreting the performance have to be used in combination, as some of the metrics such as R^2 are sensitive to outliers and few extreme errors could lead to misleading accuracy interpretation with them (Khoshvaght et al., 2025). In addition, for the analysis of the results time series plots for daily emissions as well as cumulative plots for yearly cumulative emissions are created in Matplotlib, Python (Hunter, 2007).

To report the results of different grassland systems in Germany, the model's daily N_2O-N estimations of individual soil replicates are generated and are finally aggregated on replicates of same treatment.

3 Results

3.1 Comparison of model performances

~~In this study, two architectures of LSTM were explored as shown in Fig. 2 and architecture A (Fig. 2 a) demonstrated superior performance in capturing general N_2O emission patterns compared to Architecture B (Fig. 2 b). Consequently, the final model is built on architecture A, consisting of an input layer, three LSTM layers, an attention layer, the concatenate layer to add static drivers, a dense layer, a drop out layer and an output layer. The model receives a five-day sequence of temporal drivers, alongside with two static drivers as shown in Eq. Although individual drivers show low Pearson correlation, -0.11 to 0.16 to the N_2O-N emission values in our dataset, the generated LSTM model was able to capture the influence of the interaction between all drivers to N_2O-N emission.~~

The LSTM model is built based on the architecture in Fig. 2, consisting of an input layer, three LSTM layers, an attention layer, the concatenate layer to add static drivers, a dense layer, and an output layer. The model looks at a five-day sequence of temporal drivers at each round, alongside with two static drivers as shown in Eq. 1. Although individual drivers show low Pearson correlation, between -0.11 and 0.16, to the N_2O-N emission values in our dataset, the generated LSTM model was able to capture the influence of the interaction between all drivers to N_2O-N emission.

Table 4 compares the RMSE of some of the experiments conducted in this study to identify the optimal model configuration, in which different subsets of soil properties or length of input sequences (5, 10, 20) were tested. For each experiment the hyperparameter tuning is done extensively to obtain an optimum model fitting to the input. In the current dataset, Bulk density (BD) showed strong negative Pearson correlation of -0.9 to both soil organic carbon (SOC) and clay. While all these variables are key drivers of N_2O emissions, only bulk density was included in the model due to slightly better performance in capturing emission peaks. Adding correlated features reduces model's accuracy, likely due to confusing the model with redundant features which do not provide extra

information. The results presented in next section correspond to the best-performing model in catching low and high emissions as well as cumulative emissions (index 1 in Table 4).

Index	Input soil properties	Test RMSE ($\mu g m^{-2} h^{-1}$)	Sequence length
1	**BD, pH**	**18**	**5**
2	BD, pH	23	10
3	pH, SOC	19	5
4	BD, pH	19	20
5	SOC, BD, Clay, pH	20	5

Table 4 Model specifications of 5 experiments compared in this study. The models are compared on the basis of the RMSE on the temporal test set and cross-site test set (averaged), the static inputs they receive, and the length of the input sequence. The temporal drivers are identical between the experiments.

3.2 Model performance

~~The best model performed well in modelling daily emissions in the training set, with an RMSE of 34 $\mu g m^{-2} h^{-1}$ and a relative RMSE of 200%. The model is also able to successfully estimate daily N_2O emissions in the test set, with an RMSE of 18 $\mu g m^{-2} h^{-1}$, a relative RMSE of 270% and total bias of -12%. Having relative RMSE higher than 1 is a known effect of the imbalanced dataset. Figure 3 Shows the scatter plots of model performance on the training set, the test set.~~

~~The model successfully captures the temporal fluctuations and magnitude of N_2O emissions at the test sites in various instances, although the accuracy varies between soils as shown in Fig. 4. For most sites, the general emission pattern is simulated with a high degree of accuracy. However, in some cases, there is evidence of over- or underestimation of the magnitude of N_2O emissions. For example, at Chamau and Fendt, the model predicted the overall variability of the emissions well, indicating that Chamau experiences higher peaks than other sites; however, in some cases the peak values were not accurately simulated (Fig. 4 a, b and c). At Graswang, the model tended to underestimate fluxes (Fig 4. d).~~

~~To assess the generalisability of the model, the Rottenbuch soils (at the Fendt climate) were excluded from the training set and considered as independent test soils. These soils showed variable emissions across years, with peak fluxes exceeding 150 $\mu g\ m^{-2}\ h^{-1}$ during warmer periods, particularly following fertilization events in 2015 and 2016 (Fig. 4 h and i), for which the model captures the patterns in most cases. On the other hand, fertilization during warmer periods in 2017 and 2019 did not result in elevated fluxes, and the model shows significant errors for estimating this behaviour in several cases (Fig. 4 j and k). In general, the results show that N_2O emissions are generally lower during colder seasons, and even fertilization during cold conditions does not lead to highly elevated fluxes; a pattern which is captured well by the model in most cases.~~

~~Figure 5 shows the comparison between observed and modelled annual cumulative emissions achieved by aggregating the daily fluxes. The results show that the model creates an accurate estimation of annual emissions for some soils and in different years with a slight error rate, such as Rottenbuch in Fendt 2015 intensive and Rottenbuch in Fendt 2015, 2016, 2017 extensive. But, higher overestimation on annual total emissions are evident for soils such as Rottenbuch in Fendt 2016, 2017, 2020 intensive as well as Chamau (Fig. 5 a and b).~~

The best model performed well in modelling emissions in the training set with RMSE of 34 $\mu g\ m^{-2}\ h^{-1}$, R^2 of 0.60 and a low negative bias of -5 $\mu g m^{-2} h^{-1}$ (Table 5). In this section we discuss the performance of the model in detail.

	Log scale						Original scale					
	R2	Spearman ρ	Spearman_CI 95%	RMSE	MAE	Bias	R2	Spearman ρ	Spearman_CI 95%	RMSE	MAE	Bias
Train set	0.60	0.62	[0.61, 0.63]	0.65	0.54	0.007	0.51	0.62	[0.61, 0.63]	34	10	-5
Temporal test	0.40	0.57	[0.55, 0.58]	0.70	0.53	0.32	0.35	0.57	[0.55, 0.58]	27	9	2
Cross-site test	-0.09	0.38	[0.36, 0.39]	0.70	0.58	0.36	-0.11	0.38	[0.36, 0.39]	10	5	2

Table 5. Statistics for train, temporal test and cross-site test datasets on the log scale and the original scale for the best model (index 1 in Table 4). RMSE, MAE and bias values in original scale are reported in $\mu g\ m^{-2}\ h^{-1}$ unit.

As discussed in previous sections, model training and evaluation were conducted in log space to stabilize variance and prevent extreme observations from dominating error metrics. While log-transformation improves the model's performance, it makes the interpretation of the results more challenging (Hodson,

2022). Consequently, performance metrics are reported on both the log scale and the original scale (Table 5). In the following sections, we primarily discuss results on the original scale to better reflect predictive behaviour.

Temporal test set model performance

To evaluate temporal generalization within sites, model performance was assessed on independent hold-out years not used for training. For the temporal test set the Spearman's rank correlation (ρ), reflecting the strength of the monotonic relationship between observed and predicted values, was 0.57 (95% CI [0.55–0.58]) indicating robust generalization with no evidence of overfitting (Prion and Haerling, 2014). The narrow confidence intervals across datasets among all training, temporal test as well as cross-site test sets demonstrate that these estimates are statistically stable and precise (Ruscio, 2008). Despite some performance degradation comparing to the training set, the preserved rank correlation shows that the model reliably captures the temporal ordering of emission events across years within the same sites.

The R^2 value representing the proportion of explained variance, was 0.35 for the temporal test set (Table 5), lower than in the training data (0.51). This indicates that a substantial fraction of observed variability is retained under temporal extrapolation. The model successfully captures the temporal fluctuations and, in many cases, the emission magnitudes although performance varies between soils (Fig. 4). For most sites, the general emission pattern is simulated with good agreement (Fig. 4). At Chamau and Fendt, the model predicted the overall variability of the emissions well, indicating that Chamau experiences higher peaks than other sites (Fig. 4 a, b), while individual peak magnitudes were occasionally over- or underestimated or slightly delayed. At Graswang, fluxes were more frequently overestimated (Fig. 4 c, d). These deviations in peak magnitude and timing account for the reduction in R^2.

Bias for the temporal test set was +2 μg m^{-2} h^{-1}, indicating a slight overall overestimation. Given the magnitude of observed peak fluxes, this systematic deviation is small and suggests minor systematic errors under temporal extrapolation.

The RMSE of 27 μg m^{-2} h^{-1} quantifies the average prediction error, with greater weight assigned to large deviations. Together with an MAE of 9 μg m^{-2} h^{-1}, these metrics indicate moderate errors.

Overall, the temporal test results demonstrate good generalization across years within the same sites. While some reduction in explained variance and peak accuracy occurs, the preserved rank correlation, narrow confidence interval, positive R^2, and low bias indicate robust temporal transferability.

Cross-site model performance

The cross-site evaluation is based on an independent hold-out set, comprising a soil not used during model training, thereby providing a reliable test of spatial generalizability. Spearman's rank correlation (ρ) was 0.38 (95% CI [0.36–0.39]), indicating a moderate, statistically precise monotonic relationship which is lower than the observed value for the temporal test set. Although reduced, the correlation remains statistically robust indicated by the narrow confidence intervals. Fig. 4 e–n shows that the model captures the general temporal dynamics of daily fluxes in many cases. Thus, the underlying predictive signal is preserved even under spatial transfer.

The R^2 value was negative for the cross-site test set (Table 5). This does not imply a loss of predictive skill but rather reflects the sensitivity of R^2 to a few large errors, such as extreme overestimations at Rottenbuch in Fendt during the 2017 intensive campaign following fertilization (Fig. 4 l), as even a few extreme residuals reduce R^2 significantly.

Across years, peak fluxes exceeded 150 μg m^{-2} h^{-1} during warmer periods following fertilization in 2015 and 2016 (Fig. 4 j, k), where the model generally captured timing and peak structure. In contrast, fertilization during warm periods in 2017 and 2020 did not produce elevated fluxes, yet the model simulated pronounced peaks in several cases (Fig. 4 l, n), contributing substantially to the reduced R^2. In general, the results show that N_2O-N emissions are generally lower during colder seasons, and even fertilization during cold conditions does not lead to highly elevated fluxes; a seasonal pattern which is captured well by the model in most cases. Bias for the cross-site test set was +2 μg m^{-2} h^{-1}, indicating slight overestimation and a magnitude similar to that observed for the temporal test.

The RMSE of 10 μg m^{-2} h^{-1} and MAE of 5 μg m^{-2} h^{-1} reflects the average magnitude of prediction errors but is strongly influenced by a few extreme misestimations, particularly overpredicted post-fertilization peaks in some instances. Consequently, RMSE and R^2 suggest moderate spatial generalizability.

Overall, the model retains skill in capturing temporal ordering and seasonal dynamics in many instances. Cross-site transfer reveals limitations in accurately estimating peak magnitudes under some fertilization events, while in many cases the timing and pattern of emissions are properly captured (Fig. 4 f, h, j, k).

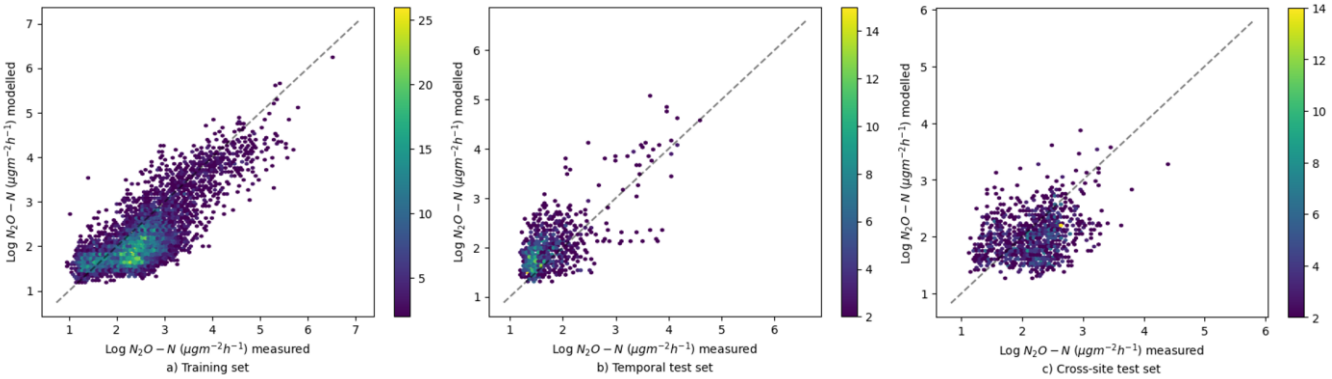


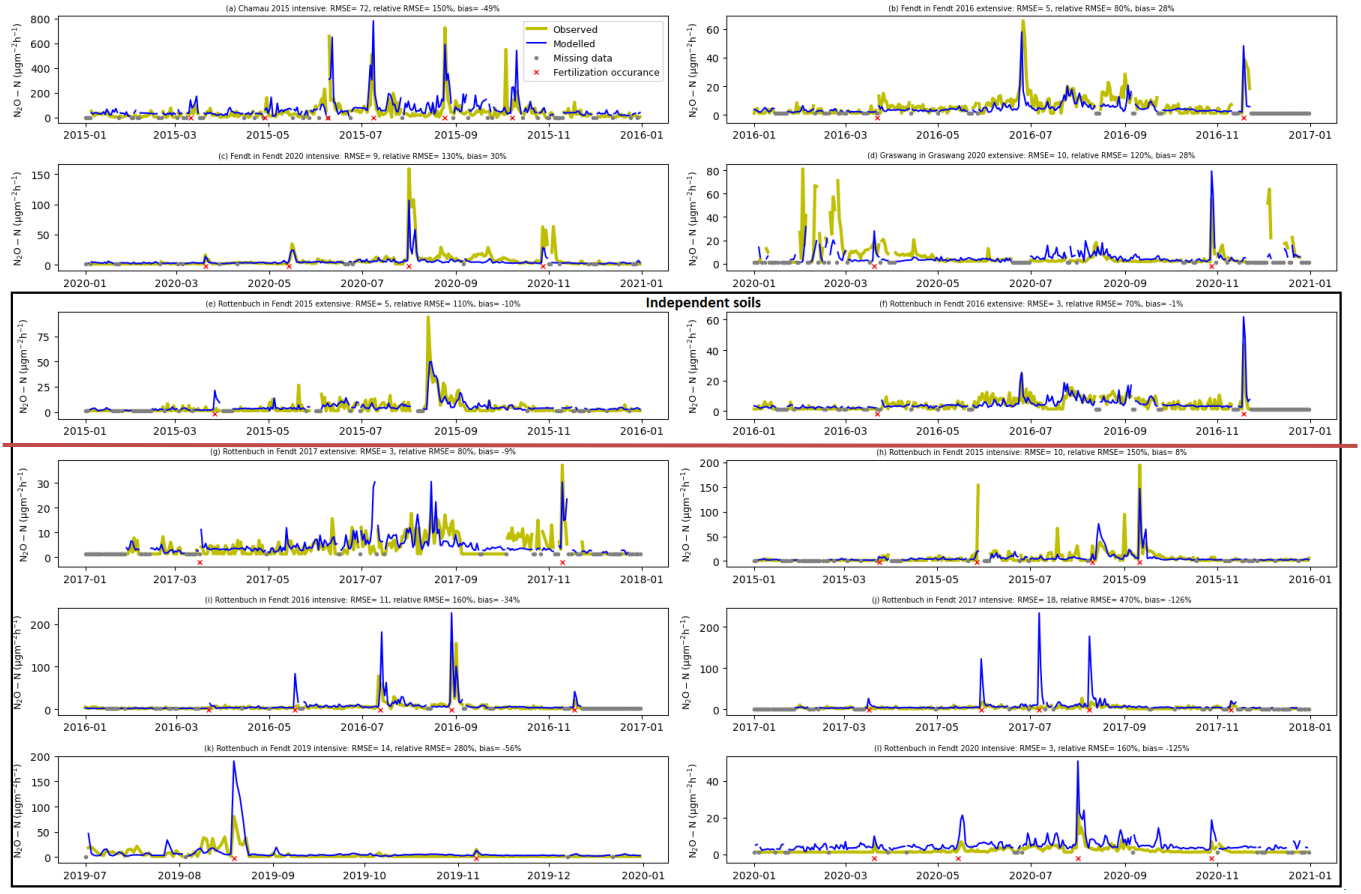
Figure 3 Hexbin plots with density colour bar comparing observed (x-axis) with simulated (y-axis) daily N_2O-N fluxes on a natural log (ln) scale for (a) the training set and (b) the temporal test set, (c) cross-site test soils of Rottenbuch in Fendt. Hexagon colors show the number of predictions falling into them, appearing as lighter (yellow) colors for bins with more data points and darker colors (blue) with less data points.

3.4 Permutation feature importance (PFI)

~~Three configurations of PFI analysis were performed on the test set to provide a comprehensive assessment of the relative importance of individual drivers. In the first configuration, PFI was applied on the entire test dataset. This analysis revealed that soil temperature at a depth of 10 cm was the most influential feature, followed by soil pH and fertilization (Fig. 6 a) while all other input features also show a high relative importance. In the second configuration, PFI was applied to individual sites in the test set in order to investigate the the importance of different drivers at site-scale N2O dynamics. The results indicate that at most sites all temporal drivers were the highly important features for N_2O dynamics (Fig. 6 b-f). However, at the Graswang site BD and pH show a very high importance, together with soil temperature (Fig. 6 d), due to high variability in soil properties within the soil cores of this grassland which affect their N2O emission (Table 2). Compared to the soil lysimeter systems in Germany including a diverse set of soils with variability in pH and BD, there is only one soil type included at the Chamau site which explains the zero relative importance of these variables at Chamau in Fig. 6 b.~~

~~In an additional analysis, we studied the varying importance of features across the five-time steps individually, shown in Fig. 7, which further highlights the role of dynamic environmental conditions in driving emissions and reinforces the need to incorporate temporal variability in emission modeling frameworks.~~

PFI analysis was performed on different soils in the test set to provide a comprehensive assessment of the relative importance of individual drivers. The results indicate that, for most soils, all temporal drivers were highly important for explaining N_2O dynamics (Fig. 6). This analysis revealed that soil temperature at 10 cm depth as well as fertilization were the most influential features in many soils while all other input features also showed a high relative importance (Fig. 6 a, b, e, f). In contrast, at Graswang in Fendt soils, BD and pH show a very high importance (Fig. 6 c and d), due to high variability in soil properties within the soil lysimeters which cause varying N_2O emission rates (Table 2). Compared to the soil lysimeter systems in Germany including a diverse set of soils with variability in pH and BD, the absence of variability in these properties at Chamau precludes their evaluation as potential drivers by PFI, which is reflected in the zero relative importance calculated for them by PFI as shown in Fig. 6a.



375 ~~Figure 4 Time series of observed and modelled N_2O fluxes in different soils at different climates and years for the test set including RMSE, relative RMSE and bias for individual soils. Note that the axis scales differ between panels to enable visibility of the data and visualize the differences between N_2O emission rates at different sites in the experiment.~~

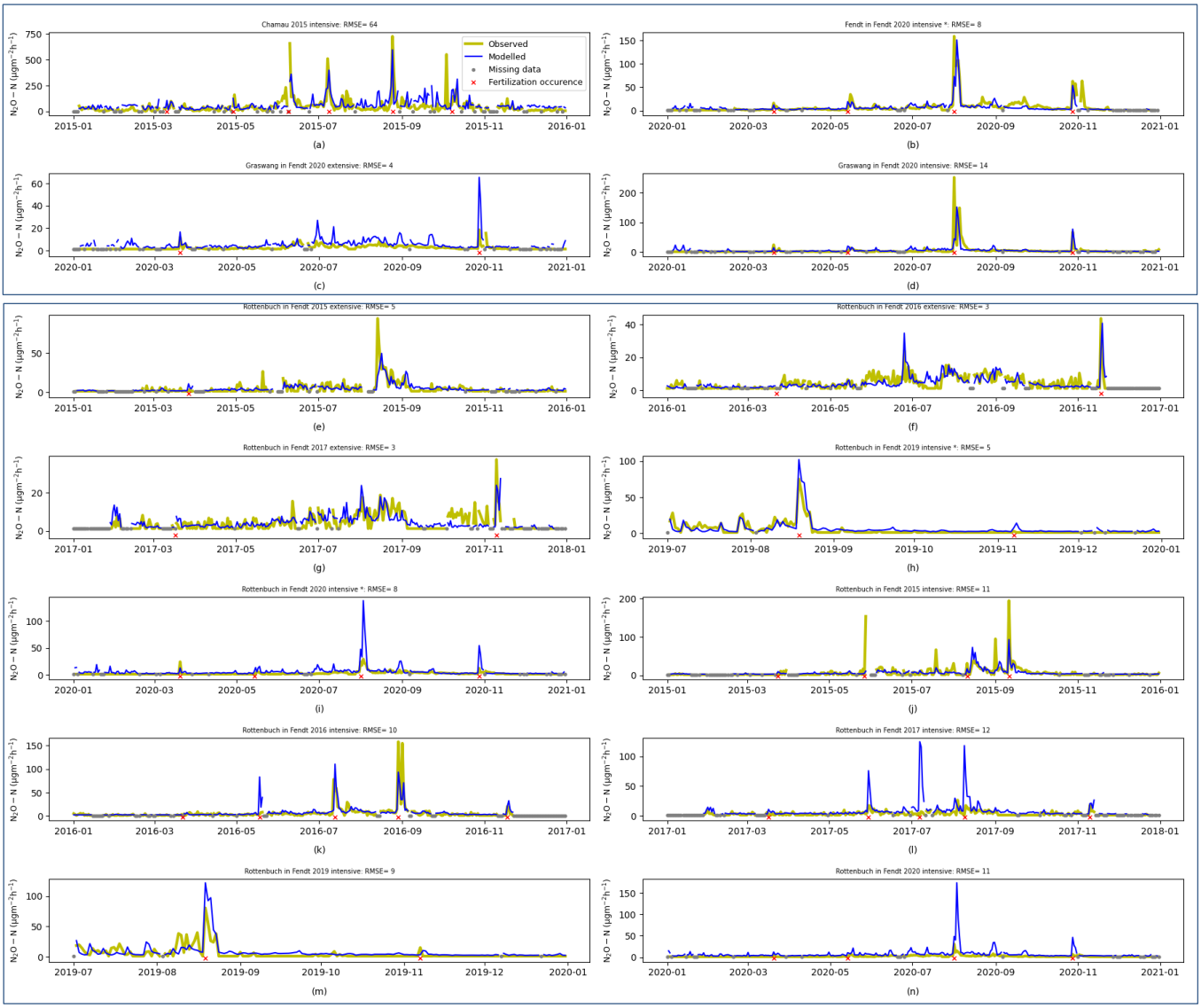
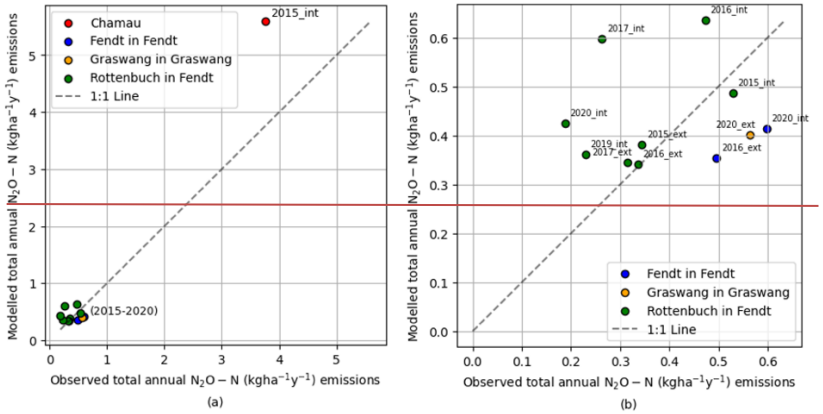
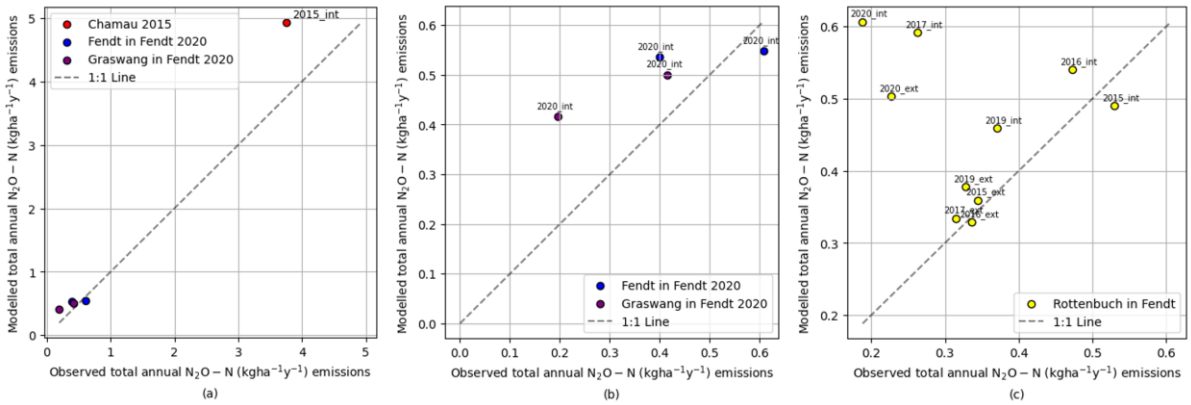


Figure 4 Time series of observed and modelled N_2O-N fluxes in different soils at different climates and years for the test set including RMSE for individual soils in a-n panels. Panels a-d show the temporal test set and panels d-n show the cross-site test sets. Note that the axis scales differ between panels to enable visibility of the data and visualize the differences between N_2O-N emission rates at different sites in the experiment. *originally managed extensively, and changed to intensive in 2019 and 2020.



385 ~~Figure 5 Cumulative observed and modelled annual N_2O emissions across multiple years for different sites representing various soils in climates: (a) all soils combined (b) enlarged version showing only the German soils including the independent test soil, Rottenbuch in Fendt.~~



390 Figure 5 Cumulative observed and modelled annual N_2O-N emissions across multiple years for different soils: (a) temporal test (b) enlarged version showing only the German soils in temporal test, (c) cross-site test set (Rottenbuch in Fendt soils). Cumulative N_2O-N fluxes were calculated using only days with available observations and the corresponding simulated values, avoiding bias from gap-filling.

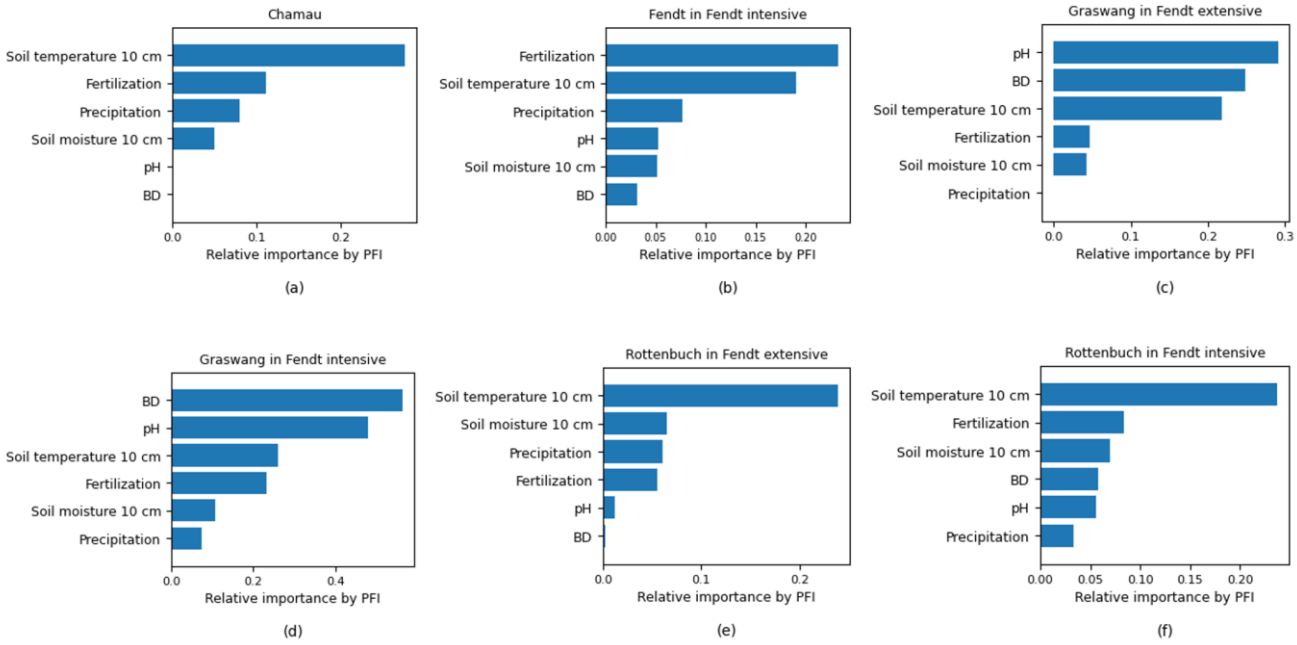
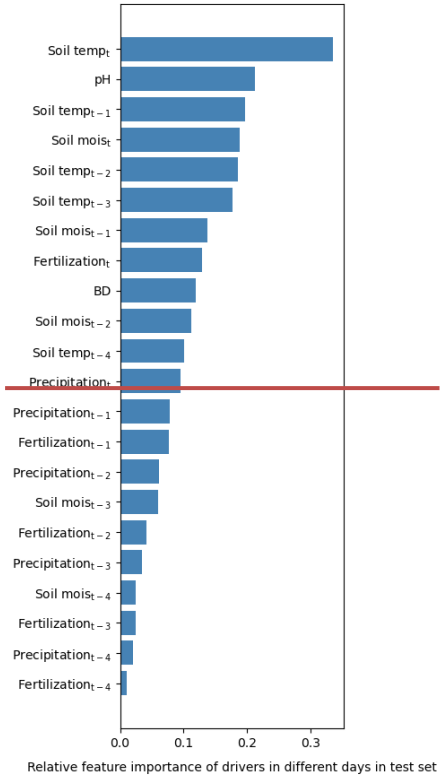


Figure 6 Relative feature importance (x-axis) of drivers (y-axis) in the test set based on MSE calculated by PFI for individual soils in panels a-f.



395 ~~Figure 7 PFI feature importance at individual days, in which t index shows the current day~~

4 Discussion

In this study, a long short-term memory (LSTM) neural network was employed to model daily N_2O emissions from grasslands in Central Europe, based on soil properties as well as key environmental and management drivers over a 5-days window.

~~Our study makes a novel contribution to simulating soil N2O emission from grassland soils using ML approaches. This is achieved by building a comprehensive problem setup, collecting a large and diverse dataset of 28,000 data points which encompasses a wide range of soil properties and climatic conditions (Table 1 and 2), incorporating an independent test site, and accounting for the role of environmental changes on N_2O emissions within several days in a sequential setup modelled by the LSTM. By contrast, recent studies (Table 5) which used ML to model GHG emissions have generally relied on smaller datasets from single sites and many of them used classical machine learning approaches with non-sequential data.~~

~~Adjuik et al. (2022) used data of variable cropping systems, sites and fertilization amendments to estimate CO_2 emissions using minimal predictors. However, train and test set split were performed randomly on the whole dataset meaning that there was no independent test site available for evaluation. Similarly, Jiang et al. (2023) collected a diverse global dataset, using 52 studies of CH_4 and N_2O from paddy fields, and applied an ensemble model combining classical ML approaches to simulate daily emissions of a single site (3 years paddy field experiment in Kushan, China) on 558 datapoints (Jiang et al., 2023). In another study, Saha et al. (2021) used a classical ML approach to model sub-daily N_2O emissions from two fertilised maize systems in the US, including an independent test site located 2 km from the training sites, but with a significantly smaller dataset and less variability in climatic conditions.~~

~~In only one other study, LSTM was used to simulate CO_2 and N_2O emissions for a single site in Quebec, Canada by Hamrani et al., 2020, and was compared with a set of ML algorithms in 3 categories: classical ML, shallow learning and other deep learning algorithms. This study demonstrated that only the LSTM model was able to provide a good prediction of N_2O fluxes, and was also more accurate than the process-based Root Zone Water Quality Model (Hamrani et al., 2020).~~

Numerous studies have modelled N_2O emissions from soils, concerning field-scale simulations across different land-use types (Saha et al., 2021; Hamrani et al., 2020; Jiang et al., 2023), regional or global modeling of emissions (Jiang et al., 2023; Adjuik et al., 2022), or knowledge-guided modeling which combines mechanistic scientific knowledge with data-driven ML to improve predictions, interpretability, and generalization compared with using either purely data-driven ML or purely mechanistic models alone (Xu et al., 2022). A summary of these studies is given in Table 6. To further advance this field and address a key methodological gap, i.e. the limited availability of rich and diverse real-world datasets enabling spatial scaling, we expanded the modeling scope to a wide regional level for grasslands across Central Europe. In addition to temporal out-of-sample testing, the model was evaluated using a cross-site approach on an independent soil dataset to assess spatial transferability. This was achieved through a comprehensive modeling framework, the compilation of a large and diverse dataset comprising 26,500 observations, and covering a wide range of soil properties and climatic conditions (Tables 1 and 2). Furthermore, short-term environmental controls on N_2O emissions were explicitly represented using a sequential LSTM model. The resulting regional model facilitates more efficient upscaling of grassland N_2O simulations within the region, without the need for site-specific parametrization which has not previously been addressed at this scale.

Study	Gas	Data source	Data size	Input drivers	Land type	ML algorithms
Current study	N_2O	-Germany, Switzerland, Austria -10 years	28000	Soil temperature, soil moisture, precipitation, occurrence of fertilization, soil pH, soil BD	Grassland	-LSTM (deep learning)
Xu et al., 2022	N_2O	Controlled mesocosm chambers	Millions synthetic, hundreds real	Soil temperature, soil moisture, soil oxygen status, soil organic carbon, dissolved organic carbon, soil ammonium, soil nitrate, air temperature, precipitation, evapotranspiration, water balance variables, fertilizer nitrogen input, fertilization timing	Cropland	KGML
Adjuik et al., 2022	CO_2	Multiple sites from GRACENET	7863	Soil temperature, Air temperature, fertilizer amendment class, soil classification, and crop type	Cropland	-Random forest -Support vector regression -Gradient boosting (best)
Jiang et al., 2023	CH_4, N_2O	-Kunshan, China -Three years	CH_4: 552 N_2O: 558	Soil temperature, soil moisture or Irrigation volume, air temperature (maximum, minimum, and average), soil redox potential, rainfall, wind speed, and radiation	Paddy fields	-Random forest -K-nearest neighbours -Gradient boosting -Linear regression -Ensemble model of all (best)
Jiang et al., 2023	CH_4, N_2O	-Cumulative fluxes global dataset collected from 52 studies	CH_4: ~60 N_2O: ~60	Soil organic carbon, pH, texture, inorganic nitrogen fertilizer application, and non-flooded days	Paddy fields	-Ensemble model of random forest, k-nearest neighbours, gradient boosting and linear regression
Saha et al., 2021	N_2O	-2 sites in US Midwest -Six years	2246	Soil moisture, air temperature, days after fertilization, soil texture, soil carbon, precipitation, nitrogen (N) fertilizer rate or inorganic N availability in the soil	Corn rotation	-Random forest model in conjunction with a process-based model (SALUS)
Hamrani et al., 2020	CO_2, N_2O	-Quebec, Canada -Five years	126	soil temperature, soil volumetric water content, air temperature, precipitation and humidity, wind speed, surface pressure, and crop nitrogen uptake	Drainage and water table management research site	-LSTM (deep learning) -Random forest (classical ML) -Feed-forward neural networks (shallow learning)

Table 6 Review of several studies which applied different ML approaches for modelling soil N_2O emissions

4.2 Model performance and role of input drivers

~~Analysis of the dataset revealed the interaction between the selected input variables for the model. For instance, even under favourable temperature conditions (warmer periods), fertilization alone did not consistently result in immediate N_2O peaks, which suggests that increased nitrogen availability, leads to increased emissions only when also other environmental conditions such as soil moisture are conducive. Another important aspect about the N_2O emissions is that the duration of elevated emissions is influenced by the interplay of environmental variables. For example, Fig. 4 c, h and j show instances of continued changes in N_2O emission magnitudes extending over multiple days following fertilization events at different soils in August which is also captured by the LSTM model.~~

The model performance statistics are shown in Table 5 in both the logarithmic and the original scale. Due to the nonlinear back-transformation from the logarithmic scale, small prediction errors in log space can translate into larger absolute deviations on the original scale. Log-transformation as a variance stabilization function is an essential step to scale the highly skewed dataset, where rare but extremely high observations can dominate the training and lead to model instability. To further address this issue, a weighted loss function (Eqs. 3 and 4) was applied to ensure that the model learns both high and low fluxes,

which would otherwise be challenging due to the imbalanced dataset shown in Fig. 1. Analysis of the dataset revealed the interaction between the selected input variables for the model. For instance, even under favorable temperature conditions (warmer periods), fertilization alone did not consistently result in immediate N_2O peaks, which is in line with the fact that increased nitrogen availability affects the magnitude, timing as well as duration of the N_2O emissions through interactions with multiple environmental conditions, such soil moisture conditions that regulate microbial processes (Wang et al., 2021; Cui et al., 2024; Butterbach-Bahl et al., 2013). For example, Fig. 4 b, h and j show instances of continued or delayed N_2O high fluxes extending over multiple days following fertilization events at different soils in August, which is also captured by the LSTM model.

~~In addition to the emission peaks following fertilization, several high peaks were observed on days with no fertilization, such as in Fendt in Fendt extensive in June 2016 (Fig. 4 b) as well as Graswang in Graswang extensive in January 2020 (Fig. 4 d). In the first case, the model successfully simulated the peak (earlier timing) caused by changes in the soil temperature in conductive soil moisture, but in the latter one the model simulated fluctuations but underestimated the magnitudes of the peaks.~~

In addition to the emission peaks following fertilization in the current dataset, several high peaks were caused by other climatic conditions, such as rewetting, which is an important driver of N_2O emissions (Butterbach-Bahl et al., 2013; Guo et al., 2014). For instance, at Rottenbuch in Fendt extensive in August 2015 (Fig. 4 e) as well as at Chamau intensive in October 2015 (Fig. 4 a) emission peaks were caused by 18 mm precipitation after 12 days of dry conditions and 5mm precipitation after 10 days of dry conditions, respectively. The model successfully simulated the occurrence and duration of the emission peaks at Rottenbuch but failed to capture the magnitude and exact timing (Fig. 4e), while at Chamau the model was unable to detect the occurrence of high emission. The detection of the pattern in the cross-site Rottenbuch soil shows a promising performance. However, further improvements—particularly through expansion of the training dataset—could enhance the model's ability to capture such episodic events more robustly.

Although the model captures daily fluctuations in many cases, inaccuracies remain in periods of very low fluxes, such as Rottenbuch in Fendt extensive in October 2017 (Fig. 4 g). During this period, changes in soil moisture, temperature and precipitation were minimal, resulting in limited variability in the driving variables and consequently reduced predicted dynamics.

During model development, we conducted a series of experiments to assess the impact of input sequence length and feature selection on model performance. Ssequence lengths of 5, 10 and 20 days were tested. While longer sequences have the potential to capture long-term soil processes, their benefits were not evident in the current dataset, likely due to the dataset's limited occurrence of such events. For example, in the current dataset there are very rare cases where the high peaks after fertilizations occur later than 5 days. This suggests that the value of longer sequences may become more apparent when they are applied to larger and more diverse datasets. We also tested an expanded feature set to incorporate other important drivers of N_2O emissions such as the rate of fertilizer nitrogen (total or inorganic N), which did not improve the results due limited variability across sites and events in the current dataset, offering little additional information to improve predictive accuracy. However, if the model is to be applied to sites with more variable fertilizer practices, including explicit N application rates would likely enhance model performance.

4.3 Feature importance analysis

The PFI analysis conducted for individual soils in the test set, consistently demonstrates that all input features contribute significantly to model performance (Fig. 6). The substantial importance of both soil and meteorological features indicates that the model captured not only the meteorological effects, but also the influence of soil parameters on N_2O emissions. Among the predictors, soil temperature ranks the most important feature which aligns with previous studies highlighting its critical role in regulating microbial processes (Wang et al., 2021; Butterbach-Bahl et al., 2013; Hamrani et al., 2020). Although soil temperature measurements are not always available at many monitoring sites worldwide, maximum air temperature can serve as a suitable proxy when strongly correlated with soil temperature. In the present dataset, the Pearson correlation between these variables is 0.86, suggesting that air temperature could be used with minimal impact on model performance.

In the current dataset, fertilization events lead to pronounced short-term peaks in emissions, and show high importance in the PFI analysis, particularly in intensively managed soils. Figure 4 demonstrates that the model effectively captures these fertilization-induced emission peaks across soils. However, because such events are relatively infrequent in the studied soils, occurring only a few times per year, it ranks lower compared to more consistently present features (Fig. 6). This reflects a known limitation of permutation feature importance, which evaluates the expected degradation in predictive performance across the full data distribution and may therefore underestimate predictors whose effects occur mainly in rare or event-driven situations.

Soil pH and BD also appear as key drivers in the PFI analyses as shown in Fig. 6, indicating that their influence on N_2O emissions is captured by the LSTM model. This is in line with the previous studies about the influence of these two variables on soil N_2O emissions (Wang et al., 2021; Butterbach-Bahl et al., 2013). BD serves as a proxy for soil porosity and compaction, factors that strongly influence oxygen availability and thereby regulate microbial processes such as nitrification and denitrification (Li et al., 2024; Butterbach-Bahl et al., 2013). Moreover, soil pH also affects the microbial processes as near neutral soil pH values (6.6 - 8.3) are optimal for denitrification (Šimek et al., 2002), while low soil pH (<5.5) inhibits N_2O reductase, the enzyme that converts N_2O to N_2 during denitrification (Samad et al., 2016). Consequently, including soil properties such as pH and BD is essential when modelling N_2O emissions (Žurovec, O., et al., 2021; Costa Jr., C., et al., 2021).

These results indicate that the LSTM model implicitly captures the environmental controls governing the balance between nitrification and denitrification processes in soils. In particular, the combined importance of temperature, soil moisture, and oxygen-related soil properties suggests that the model learns the environmental conditions under which microbial pathways leading to N_2O production are activated.

Despite their lower rank at some soils, soil moisture and precipitation remain influential showing considerable relative importance, suggesting their added value for estimating N_2O emissions (Fig. 6). A larger dataset encompassing a wider range of emission responses to these drivers would likely further highlight their role. In addition, soil moisture often varies only slowly over extended periods, which can reduce the apparent effect detected by permutation-based importance methods. This represents a known limitation of PFI, as features with limited short-term variability may appear less important than their true mechanistic influence would suggest.

4.4 Implications and limitations

The performance of the LSTM model in capturing daily emission of the test set suggests that the model has potential for both gap-filling and predictive applications in similar alpine grassland environments, with possible utility for upscaling emissions across comparable regions. However, several limitations should be acknowledged. A key challenge with LSTM models lies in their limited interpretability compared with non-recurrent models due to complex recurrent structure. Moreover, the dataset exhibits a class imbalance, as it includes infrequent but high-magnitude emission peaks alongside prolonged periods of low emissions. This imbalance complicates the model's ability to learn the drivers of emissions, requiring more complex model implementation techniques. Additionally, the number of available sub-daily flux measurements varied across days in Tereno and Chamau non-gap-filled datasets. The reason is that many gaps in N_2O measurements arise from quality control procedures and instrumental failures (Kiese et al., 2018; Feigenwinter et al., 2023). Such uneven data availability across different days introduces a bias into flux estimation modelling (Lucas-Moffat et al., 2022; Teng et al., 2020).

While this and several other studies have demonstrated the promise of machine learning (ML) models for simulating soil greenhouse gas (GHG) emissions, the full potential of these approaches remains underexplored. We identify three key directions for future research that could further advance the application of ML in this domain. Firstly, expanding the dataset to encompass more geographically and climatically diverse sites with longer term interactions between the emission drivers, along with a wider range of management practices would allow for the development of more generalized N_2O emission models for grasslands across different agroecosystems. For example, grazing practices may strongly influence N_2O emission patterns but could not be systematically evaluated in this study due to limited data availability. In the current dataset, grazing occurred only during several days across three years at the Chamau site, while other sites were non-grazed. Secondly, recent advancements in deep learning models for time series forecasting, such as transformer neural networks (Vaswani et al., 2017), could be leveraged in combination with better explainable AI tools to further enhance the progress in development of the generalized model. Transformers have demonstrated significant potential in time series modelling because of their ability to capture long-range dependencies and handle multivariate data effectively (Zerveas et al., 2021). Unlike traditional recurrent models such as LSTM, transformers process entire sequences in parallel,

making them highly scalable and efficient (Vaswani et al., 2017). Finally, other versions of the machine learning models which are trained with air temperature and precipitation instead of soil temperature and moisture could be assessed using a more diverse dataset, enabling N_2O emission predictions even where direct soil measurements are missing.

5 Conclusion

This study demonstrates the effectiveness of an LSTM model in capturing temporal dynamics of daily N_2O emission data of multiple grassland sites in Central Europe, highlighting the model's suitability for predicting soil N_2O emissions. By collecting a unique dataset from a wide range of grasslands and treatments, we developed a ~~generic~~regional model capable of accurately predicting N_2O emissions across diverse conditions in central Europe. Notably, the model's performance remained robust when tested on an independent cross-site soil dataset that was not used for training, indicating good spatial transferability. This model can therefore be used not only as a gap-filling model, but also to regionally upscale emissions in pre-alpine grasslands where the required input data are available. Future research should aim to: (1) expand the dataset to include a broader and more diverse dataset, both in terms of geographic coverage and input drivers, enhancing the model's robustness and applicability at larger scales; (2) evaluate recent advances in deep learning, such as transformer models; and (3) explore the potential of KGML approaches, to further improve prediction accuracy and model interpretability

Appendix A

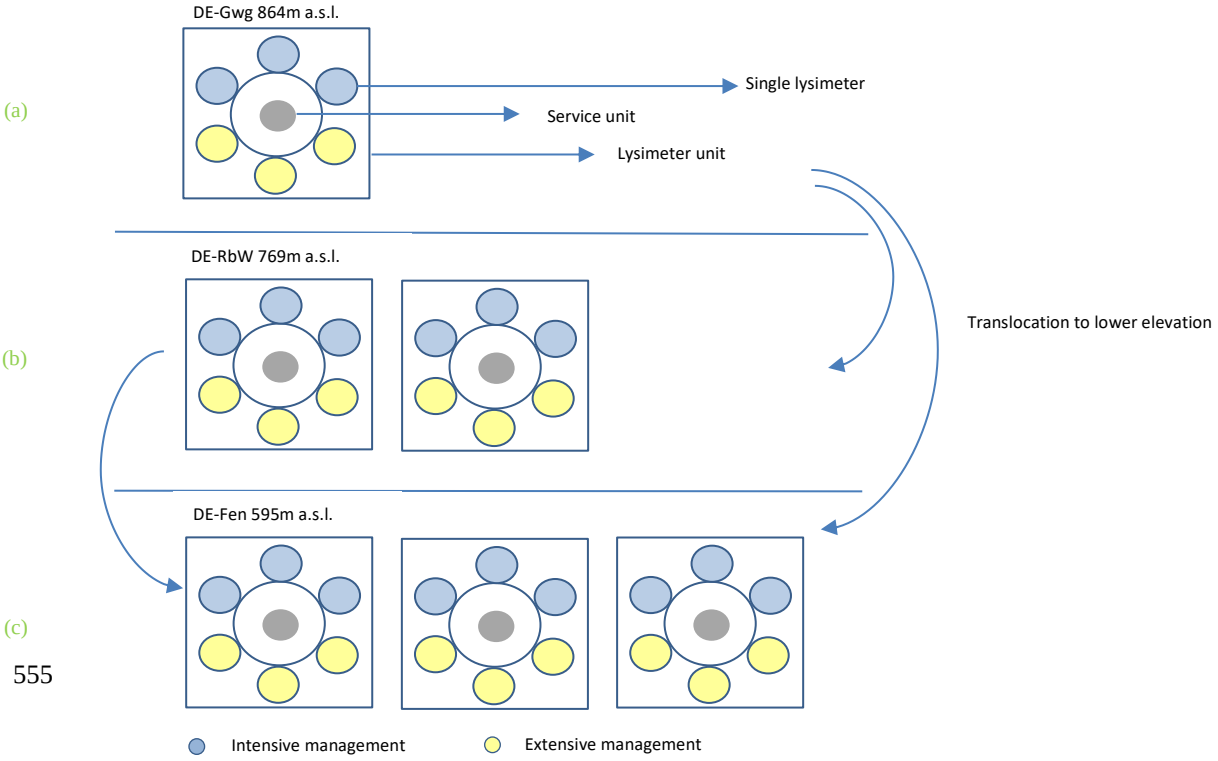


Figure A1 Scheme of lysimeter replicates originated or translocated in different grasslands, (a) Graswang (DE-Gwg), (b) Rottenbuch (DE-RbW), and (c) Fendt (DE-Fen) within the TERENO Pre-Alpine Observatory in Germany (Kiese et al., 2018).

Soil	Replicate-Management	Mean	Std	Min	Max
Neustift		20.87	6.08	7.94	37.89
Chamau		43.84	9.02	16.93	54.98
Fendt in Fendt	L1-Intensive	42.04	6.78	17.85	54.97
Fendt in Fendt	L2-Intensive	40.34	6.24	18.22	51.47
Fendt in Fendt	L3-Intensive	41.64	6.99	17.85	54.58
Fendt in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	42.96	6.67	17.85	53.90
Fendt in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	40.09	7.44	16.09	53.90
Fendt in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	43.51	7.86	17.85	54.59
Graswang in Fendt	L1-Intensive	44.44	7.22	17.28	56.14
Graswang in Fendt	L2-Intensive	43.54	6.92	19.37	53.39
Graswang in Fendt	L3-Intensive	46.25	5.90	21.01	53.56
Graswang in Fendt	L1-Extensive	45.76	7.40	19.60	57.05
Graswang in Fendt	L2-Extensive	43.64	7.04	14.90	57.65
Graswang in Fendt	L3-Extensive	40.78	6.74	19.60	54.34
Rottenbuch in Fendt	L1-Intensive	41.59	6.34	16.90	51.03
Rottenbuch in Fendt	L2-Intensive	38.97	6.25	15.56	51.70
Rottenbuch in Fendt	L3-Intensive	43.36	6.58	17.07	52.79
Rottenbuch in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	41.68	5.55	17.68	50.20
Rottenbuch in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	42.42	7.13	15.94	50.67
Rottenbuch in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	44.05	7.26	17.63	53.69
Graswang in Graswang	L1-Intensive	47.15	7.80	13.38	58.15
Graswang in Graswang	L2-Intensive	46.73	5.41	18.37	53.28
Graswang in Graswang	L3-Intensive	48.05	6.20	17.28	55.53
Graswang in Graswang	L1-Extensive	47.89	5.78	16.98	55.85
Graswang in Graswang	L2-Extensive	49.08	6.42	19.37	57.94
Graswang in Graswang	L3-Extensive	47.89	5.63	21.19	55.85

(a) soil moisture statistics of the soils

Soil	Replicate-Management	Mean	Std	Min	Max
Neustift		9.36	6.76	0.31	19.41
Chamau		12.09	6.46	1.18	25.08
Fendt in Fendt	L1-Intensive	10.80	6.82	0.49	24.40
Fendt in Fendt	L2-Intensive	10.55	6.91	0.25	24.38
Fendt in Fendt	L3-Intensive	11.02	6.86	0.40	24.42
Fendt in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	10.87	6.98	0.23	25.09
Fendt in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	10.88	6.74	0.56	24.31
Fendt in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	10.92	6.91	-0.77	24.82
Graswang in Fendt	L1-Intensive	10.53	6.87	0.63	24.74
Graswang in Fendt	L2-Intensive	10.73	6.74	0.45	24.79
Graswang in Fendt	L3-Intensive	10.86	6.80	-0.44	24.59
Graswang in Fendt	L1-Extensive	10.79	6.86	0.14	24.31
Graswang in Fendt	L2-Extensive	11.42	6.66	1.02	25.14
Graswang in Fendt	L3-Extensive	10.68	6.80	-1.28	24.38
Rottenbuch in Fendt	L1-Intensive	10.83	6.72	-0.36	25.14
Rottenbuch in Fendt	L2-Intensive	11.07	6.97	-0.22	24.96
Rottenbuch in Fendt	L3-Intensive	10.75	6.76	-0.30	24.58
Rottenbuch in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	10.48	6.59	-0.26	24.92
Rottenbuch in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	11.16	6.56	0.74	24.40
Rottenbuch in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	10.82	6.68	-0.36	24.48
Graswang in Graswang	L1-Intensive	9.40	6.93	-1.35	23.06
Graswang in Graswang	L2-Intensive	8.89	6.70	-1.35	22.20
Graswang in Graswang	L3-Intensive	9.31	6.80	-1.21	22.32
Graswang in Graswang	L1-Extensive	9.34	6.64	-0.71	22.64
Graswang in Graswang	L2-Extensive	9.28	6.50	-1.06	22.18
Graswang in Graswang	L3-Extensive	9.45	6.62	-1.43	22.73

(b) soil temperature statics of the soils

Soil	Replicate-Management	Mean	Std	Min	Max
Neustift		12.54	10.41	0.11	48.86
Chamau		70.11	114.03	-739.12	1155.83
Fendt in Fendt	L1-Intensive	5.84	13.56	-25.01	248.33
Fendt in Fendt	L2-Intensive	4.52	7.79	-26.17	160.07
Fendt in Fendt	L3-Intensive	11.44	30.64	-25.68	707.50
Fendt in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	6.27	19.81	-30.72	357.82
Fendt in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	6.13	12.79	-15.00	192.32
Fendt in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	14.97	48.18	-24.85	750.38
Graswang in Fendt	L1-Intensive	7.16	35.14	-25.57	960.49
Graswang in Fendt	L2-Intensive	5.77	14.12	-26.52	288.06
Graswang in Fendt	L3-Intensive	6.10	16.39	-20.97	326.71
Graswang in Fendt	L1-Extensive	6.09	17.05	-28.28	428.09
Graswang in Fendt	L2-Extensive	4.88	8.21	-26.73	164.57
Graswang in Fendt	L3-Extensive	3.52	5.80	-27.29	79.14
Rottenbuch in Fendt	L1-Intensive	4.30	10.84	-30.25	226.26
Rottenbuch in Fendt	L2-Intensive	4.40	13.25	-22.33	275.85
Rottenbuch in Fendt	L3-Intensive	6.09	16.04	-10.27	323.24
Rottenbuch in Fendt	L1-Extensive (2014-2018), Intensive (2019-2020)	2.84	4.03	-15.93	52.58
Rottenbuch in Fendt	L2-Extensive (2014-2018), Intensive (2019-2020)	4.09	6.15	-14.12	81.62
Rottenbuch in Fendt	L3-Extensive (2014-2018), Intensive (2019-2020)	5.68	10.92	-13.35	132.58
Graswang in Graswang	L1-Intensive	14.14	36.82	0.22	513.37
Graswang in Graswang	L2-Intensive	11.78	26.53	1.19	230.11
Graswang in Graswang	L3-Intensive	9.01	22.17	-0.48	283.05
Graswang in Graswang	L1-Extensive	11.37	21.43	1.14	222.33
Graswang in Graswang	L2-Extensive	8.33	15.67	0.46	103.26
Graswang in Graswang	L3-Extensive	4.90	5.96	1.12	49.66

(c) N_2O statistics of the soils

Table A1 Statistics of the soils in different climates with respect to (a) soil moisture at 0–10 cm depth, (b) soil temperature at 0–10 cm depth, and (c) daily N_2O emissions.

Data and code availability

The datasets analyzed during the current study were sourced from existing publications. The code to the implemented LSTM model architecture in python is available under: https://github.com/Samin-Payrosangari/LSTM_N2O_emission_grasslands

Author contributions

SP conceptualization, investigation, data collection and analysis, model implementation, visualization, writing -original draft preparation, -review and editing. KF conceptualization, writing -review and editing, supervision. BW: data provision, writing -review and editing. RK: data provision, writing -review and editing, supervision. CS conceptualization, writing -review and editing, supervision, funding acquisition, project administration.

Competing interest

The authors declare that they have no competing interests.

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