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A process-based framework for national-scale estimation of agricultural soil N_2O emissions under variable climate and management

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Abstract. Agricultural soils are the dominant source of anthropogenic N_2O emissions, yet their high spatial and temporal heterogeneity provides a major challenge for accurately quantifying emissions and evaluating mitigation options. Most national greenhouse gas inventories rely on empirical Tier-1 or Tier-2 emission-factor approaches and therefore do not fully capture the effects of climate variability, soil properties, or management practices. Here, we present a transferable, process-based modelling framework based on the biogeochemical model LandscapeDNDC for determining direct and indirect N_2O emissions from major crops cultivated on mineral soils at the national scale. We apply the method to Germany making use of high-resolution input data provided by the national reporting agencies, estimating N_2O emissions of 35 (29-44) kt N yr^{-1} (2017-2022 average). This is 28% higher than the national inventory report (submission 2025), but well within the uncertainty range. In contrast to conventional inventory methods, the framework explicitly accounts for interannual climate variability and can be spatially disaggregated at high resolution, taking into account local variations in soil type, weather and agricultural management practices. Because the model simulates coupled carbon and nitrogen cycling, it also quantifies multiple nitrogen loss pathways and potential changes in carbon stocks simultaneously, providing a consistent basis for evaluating mitigation strategies and their potential trade-offs. Our results demonstrate that process-based modelling can substantially improve the spatial and temporal resolution of agricultural N_2O emissions and provide a platform for developing next-generation national greenhouse gas inventories. While further work is required before the framework fully satisfies all IPCC Tier-3 requirements, it offers a pathway towards a more mechanistic and policy-relevant assessment of agricultural greenhouse gas emissions.

Key words: N_2O emissions, agricultural soils, national reporting, process-based modelling, Tier-3, Germany

https://doi.org/10.5194/egusphere-2026-4010
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1 Introduction

Estimating sector-specific, national greenhouse gas emission fluxes is important for designing appropriate mitigation strategies and monitoring their success. Such estimates are particularly challenging for nitrous oxide (N_2O), where on a global scale anthropogenic emissions are dominated by agricultural sources, and in particular agricultural soils (Fowler et al., 2013; Scheer et al., 2020; Tian et al., 2020, 2024a). N_2O emissions from agricultural soils are highly spatially and temporally heterogeneous, due to their dependence on various microbial processes that respond non-linearly to N inputs, soil and crop type, weather and agricultural management practices (Butterbach-Bahl et al., 2013; Groffman et al., 2009). At regional to national scales, measurement efforts are inherently limited by the sampling capacity, leading to two key challenges: upscaling these measurements to generate national inventories and accurately distributing N_2O emissions across heterogenous landscapes (Ogle et al., 2020).

The most common strategy for producing national inventories of N_2O emissions involves emission factors. Measurement data is collected at a global (Tier 1) or national (Tier 2) level and a relationship is determined between N inputs and N_2O emissions (Bouwman, 1996; Bouwman et al., 2002; Philibert et al., 2012; Shcherbak et al., 2014; Stehfest and Bouwman, 2006; Van Groenigen et al., 2010). While in principle it is possible to derive a different relationship between N inputs and N_2O emissions for different soils, climates, crop types, N inputs (e.g. mineral fertiliser, manure, atmospheric deposition or crop residues) and agricultural management routines, in practice the limited availability of measurement data means that it is necessary to simplify by averaging over most of these variables (Calvo Buendia et al., 2019). Thus, even in countries that have determined emission factors on a national scale, the spatial and temporal resolution of the resulting N_2O emission fields remains coarse compared to the heterogeneity of the agricultural landscape. For example, Germany has been split into 4 climate zones, but not further subdivided (Mathivanan et al., 2021). In consequence, the emission factor approach is not able to take advantage of the increasingly available high-resolution data for agricultural activity (e.g., via remote sensing), soil type and climate. Furthermore, the low spatial and temporal resolution makes it inappropriate as a base for developing detailed mitigation strategies that aim to find a trade-off between crop yields and environmental impacts. On the other hand, the relative simplicity of the approach makes it easy to apply to each new year in the annual cycle of national reporting and to project methodological changes back across the reporting period (typically 1990 until two years before reporting year).

Process-based modelling offers an alternative (Tier-3) method for determining N_2O emissions, in which higher complexity is traded against higher sensitivity to differing conditions. Process-based models aim to simulate the C and N cycling in the coupled soil-plant-atmosphere system, including the transformations between different C and N species and their physical transport. The focus on processes rather than outcomes allow them to be parametrised using a wider range of measurement data than for emission factors, and they have proved capable of estimating yields and N_2O emissions at the field scale (Grados et al., 2024; Houska et al., 2017; Molina-Herrera et al., 2016). Process-based models are thus better able to take into account

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

what is known about the heterogeneity of the agricultural landscape and produce estimates of N_2O emissions at high spatial and temporal resolution. However, due to their need for detailed input datasets and high computational requirements, they have not been widely adopted for national inventory reporting of N_2O emissions, with only the USA recently using a Tier-3 approach (EPA, 2024).

Here we present a flexible, Tier-3 framework for estimating national N_2O emissions using the process-based model LandscapeDNDC (LDNDC), and compare the results with the current methods used for national inventory reporting in Germany. The Tier-3 system performs point sampling of the agricultural landscape, stratified by grid cells. The size of the sample and the resolution of the grid can be adjusted depending on the spatial resolution of the input data (for soil, climate, agricultural management etc.) and the available computing power. The resulting N_2O emissions can also be determined at a temporal scale commensurate with the input data. This flexibility allows the framework to be adapted to a wide range of input data resolutions, making it a versatile tool for generating detailed N_2O emission inventories that can be adapted to the needs of different countries.

As an example, we use this framework to determine an inventory of N_2O emissions from agricultural soils in Germany, resolved across 403 administrative districts (European Parliament, 2024). Germany provides a good test case since it has a diverse agricultural landscape (BMLEH, 2026) that covers a large percentage of the land area (52%) and is documented at high resolution (Blickensdörfer et al., 2022; Schwieder et al., 2022). In general, there is one harvest per year and a wide range of crop types, including a large fraction of winter crops and grassland. This includes intensive grass and silage maize production in the North West, more extensively managed arable crops in the dryer North East, intensive arable agriculture across the central zone and a mixed agriculture in the south that includes both intensively managed arable and grassland and extensively managed grassland in the high pastures of the Alps. It also spans a range of climate zones (both coastal and continental) and is covered by a diverse set of soil types (Gebauer et al., 2022; Ließ, 2022; Poeplau et al., 2020; Sakhaee et al., 2022).

2 Methods

2.1 Tier-3 Model description and calibration

LDNDC is a process-based model that simulates the cycling of C, N and water in the coupled soil-plant-atmosphere system on an hourly timestep (Haas et al., 2013). It evolved out of the DNDC model (Li et al., 1992), but has since been substantially altered, for example by improving the description of the soil and plant physiological processes (Kraus et al., 2015). Here we used LDNDC revision 12410 with the submodels MeTr^x for simulating soil biogeochemical processes and associated greenhouse gas exchange (Kraus et al., 2015), PlaMo^x for plant physiology (Kraus et al., 2015; Molina-Herrera et al., 2016; Petersen et al., 2021), WatercycleDNDC for soil water transport (Kiese et al., 2011) and CanopyECM for microclimate (Grote et al., 2011).

The most important model parameters controlling the emission of N_2O from soil were calibrated using a Bayesian framework (Gurung et al., 2020, 2026; Ogle et al., 2023; Santabarbara, 2020). In the Bayesian method the aim is not to find a best model parameter set, but to find an ensemble of model parameter sets with associated likelihoods. When running national-level simulations parameter sets we sampled from this ensemble using the likelihoods as sampling weights.

The first step in the calibration was to collect high frequency N_2O measurement data from Germany and neighbouring countries (see Table D1). We aimed to collect data with daily measurements covering a full year, but also included a few studies covering only the growing season and with lower measurement frequency (e.g. 1-2 times per week). Data from 12 sites were included, many of which provide data across multiple treatments and/or years, resulting in a total of 58 treatment-years and 8799 individual measurements. This includes 41 treatment-years for croplands (22 winter wheat, 9 maize, 3 rapeseed, 2 barley, 2 cultivated grass, 1 sugar beet, 1 potato, 1 beans) and 17 treatment-years for permanent grasslands (5 extensively, 12 intensively managed), with a range of fertilisation levels and management practices. LDNDC simulations were set up for each site and treatment. For most sites data was available for crop yield, crop nitrogen content and soil water content, and small adjustments of the model species parameters and soil hydraulic properties were performed to ensure a good fit to this data.

Next, 15 of the most important model parameters that govern N_2O emissions were identified by a combination of sensitivity analysis and expert knowledge (see Table D2). This included parameters controlling the denitrification and nitrification processes, the dependence of the anaerobic volume fraction on oxygen partial pressure and the mineralisation rate of humus pools. For each of these parameters a range of possible values were defined based on the available literature. This range was then used to define a uniform prior for the Bayesian calibration. 100,000 parameter sets were drawn from the resulting parameter space using a Latin hypercube sampling method and the model was run for each site, treatment and parameter set. The parameter sets were then filtered to reduce the chances that the model gets the correct result for the wrong reasons, for example by suppressing denitrification and producing N_2O emissions only as part of the nitrification process. The requirements were: 1) a physically reasonable relationship between the anaerobic volume fraction of the soil and the oxygen partial pressure; 2) a value of $R_{N_2O} = N_2O/(N_2O + N_2) < 0.2$ when averaged across all sites, treatments and years (Kleineidam et al., 2025; Scheer et al., 2020, 2025); and 3) N_2O emissions in the range 0.5-5 $kgNha^{-1}yr^{-1}$ when averaged across all sites, treatments and years. Applying the constraints reduced the number of parameter sets to 2743. A likelihood value was then assigned to each parameter set by comparing each of the 8799 measured datapoints to the simulated values via a multivariate Gaussian function and taking a product of the associated likelihoods (see Appendix A for more details).

For each of the 2743 model parameter sets that emerged from the calibration, we performed an additional calibration step that aimed to account for uncertainty associated with the model structure and with the choice of model parameters beyond those already calibrated (Gurung et al., 2020, 2026; Ogle et al., 2010, 2007, 2023). A linear mixed effects model was constructed to

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

compare the seasonal/yearly observed and simulated emissions, with random effects used to account for correlations between measurements at the same site. The fitted model yielded a set of hyperparameters describing the distribution of predicted yearly emissions as a function of the simulated yearly emissions. For randomly sampled sites across Germany these hyperparameters were used to map the simulated emissions for a given model parameter set onto a distribution of predicted emissions, which was included in the overall uncertainty. Additional details are given in Appendix A.

2.2 Tier-3 simulation framework

The simulation framework is constructed by first defining a region of interest (e.g., Germany) and then imposing a spatial grid that defines the sub-regions within which N_2O emissions (or any other output of LDNDC) should be calculated. This grid can be administrative (e.g. districts or municipalities), square (e.g. 10×10 km grid cells) or of any other desired shape. Point-based sampling is then carried out within these grid cells, with the number of points per grid cell either uniform or proportional to the agricultural area. In this study, we used the 403 current districts of Germany as the grid (GADM v4.1, 2024), with 10,000 sampling points distributed proportional to the grid cell's agricultural areas. A LDNDC simulation was performed for the full period for every sampled point, using the best available input data (see below). Direct N_2O emissions for a grid cell were determined by averaging over the sampled points, assigning all points equal weight. Direct N_2O emissions for the region as a whole were determined by performing an agricultural-area-weighted average across grid cells. A similar approach was used to determine N leaching out of the rooting zone and gaseous emissions of NH_3 and NO, both of which may be converted to N_2O in the wider environment. Indirect N_2O emissions were determined by multiplying the N leaching and the NH_3 and NO emissions by the appropriate IPCC emission factor (Calvo Buendia et al., 2019). For NH_3 and NO we considered the difference between the volatilisation from agricultural fields and the deposition of reduced N to avoid double counting (see below for additional details).

Simulations were run for the period 2012-2022, including a 5-year spin up (2012-2016) and a 6-year core simulation (2017-2022). The simulations were driven by detailed input datasets that included crop rotation and grassland management data at 10×10m resolution (Blickensdörfer et al., 2022; Schwieder et al., 2022), fertiliser input rates resolved across 9649 municipalities in Germany (Zinnbauer et al., 2023, 2024), crop calendars at 1×1km resolution (Kaspar et al., 2014), soil data at 100×100m resolution (Gebauer et al., 2022; Poeplau et al., 2020; Sakhaee et al., 2022), climate data at 0.1×0.1° resolution (Cornes et al., 2018), N deposition data at 1×1km resolution (Kranenburg et al., 2024) and tillage data resolved across 38 districts in Germany (Eurostat, 2024). Additional assumptions were made about fertiliser distribution between crops, fertiliser timing, residue management and irrigation. More details are given in Appendix B.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

2.4 Uncertainty estimation

The uncertainty associated with the direct N_2O emissions was determined via a Monte Carlo method that combines input uncertainties, sampling uncertainties, model parameter uncertainties and model structure uncertainties (Gurung et al., 2020, 2026; Ogle et al., 2023). Here we performed 100 Monte Carlo runs, with different perturbations of the input data, a different set of sampled sites, a different model parameter set drawn from the calibration set according to the likelihoods defined above and parameter-set specific hyperparameters drawn for each simulated site. The median of the 100 Monte Carlo runs was taken as the best estimate for N_2O emissions and a 95% confidence interval was determined.

Of the many model inputs the N fertilisation rate, the soil organic matter fraction and the soil bulk density have been identified as particularly important drivers of the N_2O emissions (Santabarbara, 2020). Since the input datasets for these quantities lack an uncertainty estimate we made educated guesses for the likely uncertainty. For N fertiliser inputs we combined uncertainties at three levels: 1) the national total N input summed over the simulation period; 2) uncertainty over the year in which the N fertiliser was applied and 3) uncertainty over how it was distributed across the country. For the soil organic carbon and nitrogen and the bulk density we took into account: 1) systematic errors that result in a bias in the national dataset; and 2) measurement/propagation errors that result in site level uncertainties. The soil organic carbon and nitrogen were varied together, such that the C:N ratio remained constant. Additional details are given in the Appendix A.

The uncertainties associated with indirect N_2O emissions were determined by using a Monte Carlo method to combine the model uncertainty for N leaching and volatilisation of NH_3 and NO with the uncertainty of the IPCC emission factors. The uncertainty associated with the total (direct + indirect) N_2O emissions was similarly calculated by a Monte Carlo method that combines all the uncertainties associated with the direct and indirect emissions.

2.4 Comparison to the national inventory

The German National Inventory Document (submission 2025) describes a set of methods for determining annual N_2O emissions from agricultural soils (German Environment Agency, 2025). Here we applied these methods to the same input data used in the Tier-3 method, allowing for a direct comparison. This meant excluding emissions arising from organic soils and soils on which minor crops are cultivated (see Appendix C). As a result the N_2O emissions considered here correspond to approximately 70% of those reported in the national inventory. The correspondence is summarised in Figure 1 and additional details are given in Appendix C.

One complication in comparing the LDNDC simulations with the national inventory concerns the treatment of reactive deposition on agricultural fields and the classification of the resulting N_2O emissions as direct or indirect. In LDNDC, N deposition is one of the drivers of direct N_2O emissions, albeit a relatively minor one compared to the much larger input of N

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

fertiliser. To avoid double counting, indirect emissions were therefore calculated by taking the difference between the volatilisation of NH_3 and NO from agricultural fields and the deposition of reduced N. In the national inventory, by contrast, deposition of reactive N is not considered as a driver of direct N_2O emissions, and indirect emissions are therefore calculated from the total NH_3 and NO emissions, without subtraction of deposition. To allow for a meaningful comparison, we here reclassified part of the deposition-related national inventory emissions from indirect to direct (see Figure 1). This reclassification did not affect the total N_2O emissions reported in the national inventory.

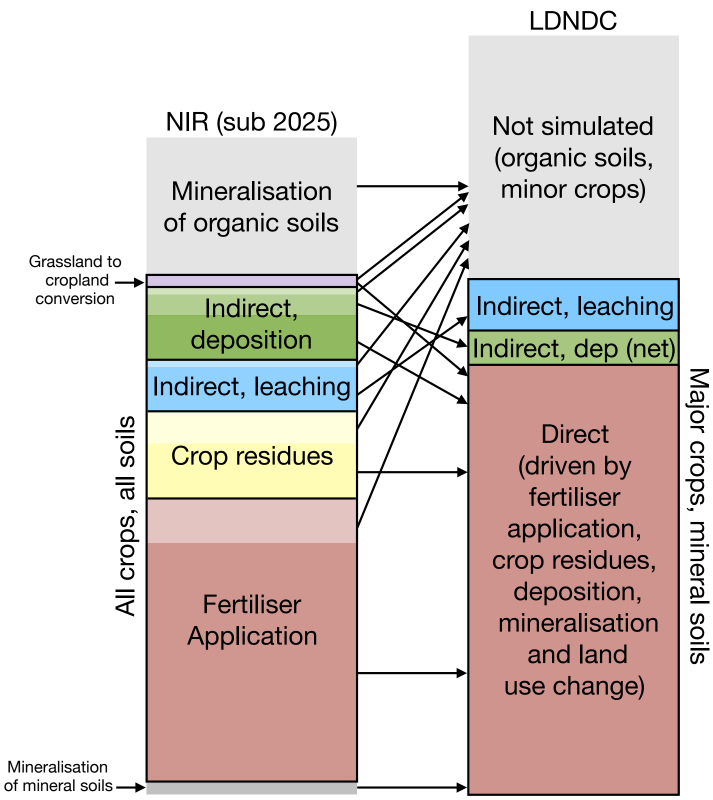

Figure 1: Correspondence between N_2O emissions reported in the National Inventory Document (NIR, submission 2025) and the Tier-3 method (LDNDC). The columns are scaled by the N_2O emission rates in 2021. The NIR bar is split into components according to the source of the N_2O emissions. These components are further split by their correspondence with the categories used in the Tier-3 method. Fertiliser application and crop residues are split into a lower part that maps onto the Tier-3 direct emissions from major crops and mineral soils and an upper part that is not simulated in the Tier-3 method (minor crops and organic soils). Indirect emissions from leaching are similarly split between indirect leaching from major crops and mineral soils, which is simulated in the Tier-3 method, and a part that is not simulated. Indirect emissions from deposition are split into three, one part that maps onto the direct emissions simulated by LDNDC, one part that maps onto the net indirect emissions from deposition and one part that is not simulated. In the Tier-3 method, net indirect emissions due to deposition are calculated from the difference between NH_3 and NO emissions and the deposition of reduced N.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

3 Results

3.1 A national inventory of N_2O emissions

The Tier-3 simulations cover an area of 14.9-15.2 Mha in the period 2017-2022 and receive 2290-2730 ktNyr^{-1} as fertiliser, corresponding to 89-91% of the total fertiliser usage in Germany. The methods used in the national inventory to calculate N_2O emissions are applied to exactly the same area and fertiliser input to allow for a fair comparison. Direct N_2O emissions in the Tier-3 method in the period 2017-2022 range from a minimum value of 25.9 (23.2-32.4) ktNyr^{-1} in 2021 to a maximum of 30.3 (26.1-37.4) ktNyr^{-1} in 2019, with an average over the period of 28.0 ktNyr^{-1} (see Figure 2). The 95%-confidence interval is 11-15% below and 16-27 % above the emission estimate. For comparison, direct N_2O emissions derived from the national inventory methods range from 20.5 (12.3-29.0) ktNyr^{-1} in 2022 to 24.4 (14.5-34.4) ktNyr^{-1} in 2017 with an average over the period of 22.2 ktNyr^{-1}. Uncertainties are 39-41% below/above the emission estimate. On average the Tier-3 method estimates 26% higher direct N_2O emissions than the national inventory methods. However, there is no statistically significant difference between the two methods, with the Tier 3 estimates lying well within the uncertainty range of the national inventory methods.

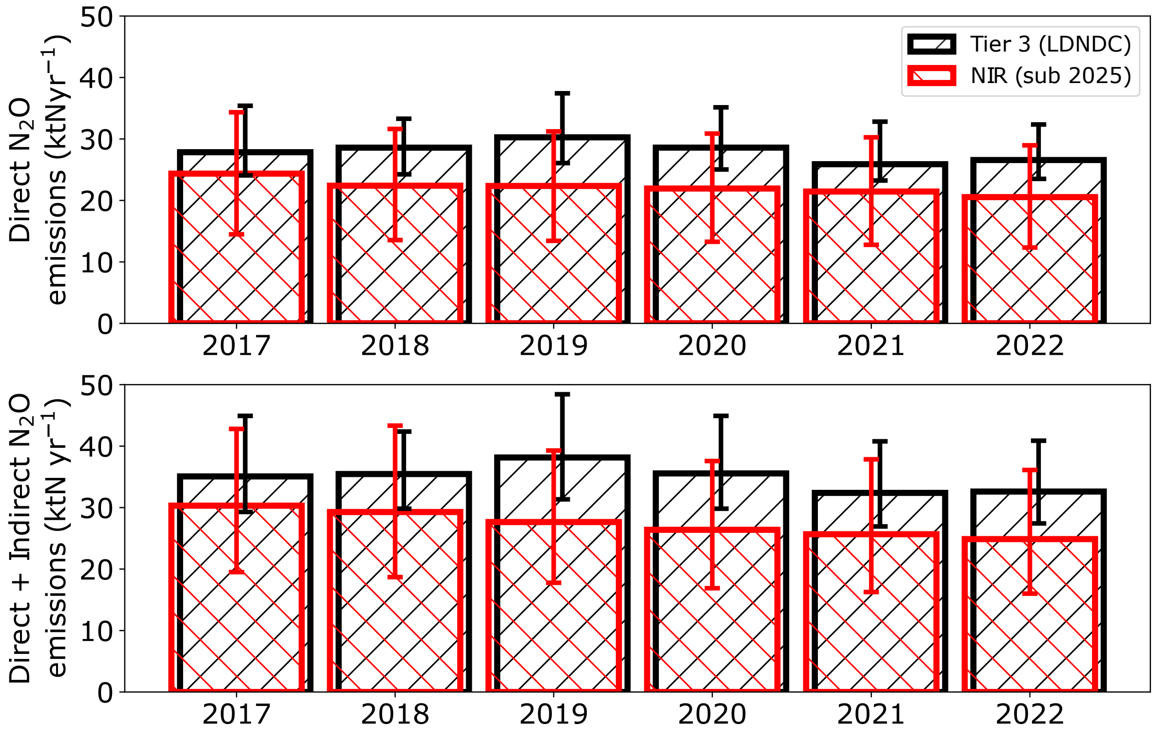

Figure 2: Yearly N_2O emissions from major crops cultivated on mineral soils in Germany. (Upper panel) Direct emissions from agricultural soils. (Lower panel) Also including indirect emissions arising from the conversion of leached N and NH_3 and NO emissions to N_2O in the wider environment. The emissions determined by the Tier-3 method are shown by black bars and the national inventory method by red bars.

Indirect N_2O emissions can be calculated from N leaching and NH_3 and NO emissions. The Tier-3 method estimates N leaching rates ranging from 124 (23-418) ktNyr^{-1} in 2018 to 277 (50-889) ktNyr^{-1} in 2021, with an average over the period of 222 ktNyr^{-}

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

^{1} (see Figure D1). This can be compared to the national inventory estimate that ranges from 222 (0-667) $ktNyr^{-1}$ in 2022 to 340 (0-1020) $ktNyr^{-1}$ in 2017, with an average over the period of 274 $ktNyr^{-1}$. The Tier-3 method estimates NH_3 and NO emission rates ranging from 276 (159-543) $ktNyr^{-1}$ in 2021 to 477 (270-788) $ktNyr^{-1}$ in 2018, with an average over the period of 382 $ktNyr^{-1}$. The national inventory estimate ranges from 216 (162-269) $ktNyr^{-1}$ in 2022 to 291 (218-364) $ktNyr^{-1}$ in 2017, with an average over the period of 250 $ktNyr^{-1}$. The annual deposition of reduced N over the period ranged from 130-158 $ktNyr^{-1}$. After excluding the deposition of reduced N, the Tier-3 method estimates indirect N_2O emissions ranging from 5.5 (2.4-10.6) $ktNyr^{-1}$ in 2022 to 7.5 (3.5-14.7) $ktNyr^{-1}$ in 2019, with an average over the period of 6.4 $ktNyr^{-1}$. For comparison the national inventory method estimates indirect N_2O emissions ranging from 3.4 (1.4-12.2) $ktNyr^{-1}$ in 2022 to 5.6 (2.2-19.2) $ktNyr^{-1}$ in 2018, with an average over the period of 4.5 $ktNyr^{-1}$.

The sum of the direct and indirect N_2O emissions is shown in Figure 2. The Tier-3 method estimates direct and indirect N_2O emissions ranging from 32.4 (26.9-40.8) $ktNyr^{-1}$ in 2021 to 38.2 (31.3-48.4) $ktNyr^{-1}$ in 2019, with an average over the period of 34.9 $ktNyr^{-1}$. Uncertainties (95% confidence interval) are 16-18% below and 19-28 % above the emission estimate. The national inventory method estimates direct and indirect N_2O emissions ranging from 24.9 (16.0-36.1) $ktNyr^{-1}$ in 2022 to 30.3 (19.5-42.8) $ktNyr^{-1}$ in 2017, with an average over the period of 27.4 $ktNyr^{-1}$. Uncertainties are 35-37% below and 41-48 % above the emission estimate. On average over the period the Tier 3 method estimates 28% higher N_2O emissions from major crops cultivated on mineral soils.

The total reported N_2O emissions from agricultural soils in the National Inventory Document (submission 2025), which also includes emissions from sources not considered in this paper (i.e. organic soils and minor crops) is 40.7 $ktNyr^{-1}$ averaged over the 2017-2022 period (German Environment Agency, 2025). The Tier-3 method developed in this paper thus accounts for approximately 70% of these emissions (67% if using the national inventory values, 72% if substituting in the Tier-3 values where applicable).

3.3 Sub-national N_2O emissions

At sub-national resolution we consider only direct N_2O emissions, since we cannot determine where the indirect N_2O emissions occur. Using the Tier-3 method we determine yearly direct N_2O emissions from mineral soils at district scale (403 districts across Germany), as shown in Figure 3. The N_2O emission rates vary between districts, ranging from 0.9-3.6 $kgNha^{-1}yr^{-1}$. The agricultural area also varies considerably between districts, ranging from a few hectares to 256 kha, leading to large differences in emissions. Higher emission rates are generally found in the North West and West and lower rates in the North East.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

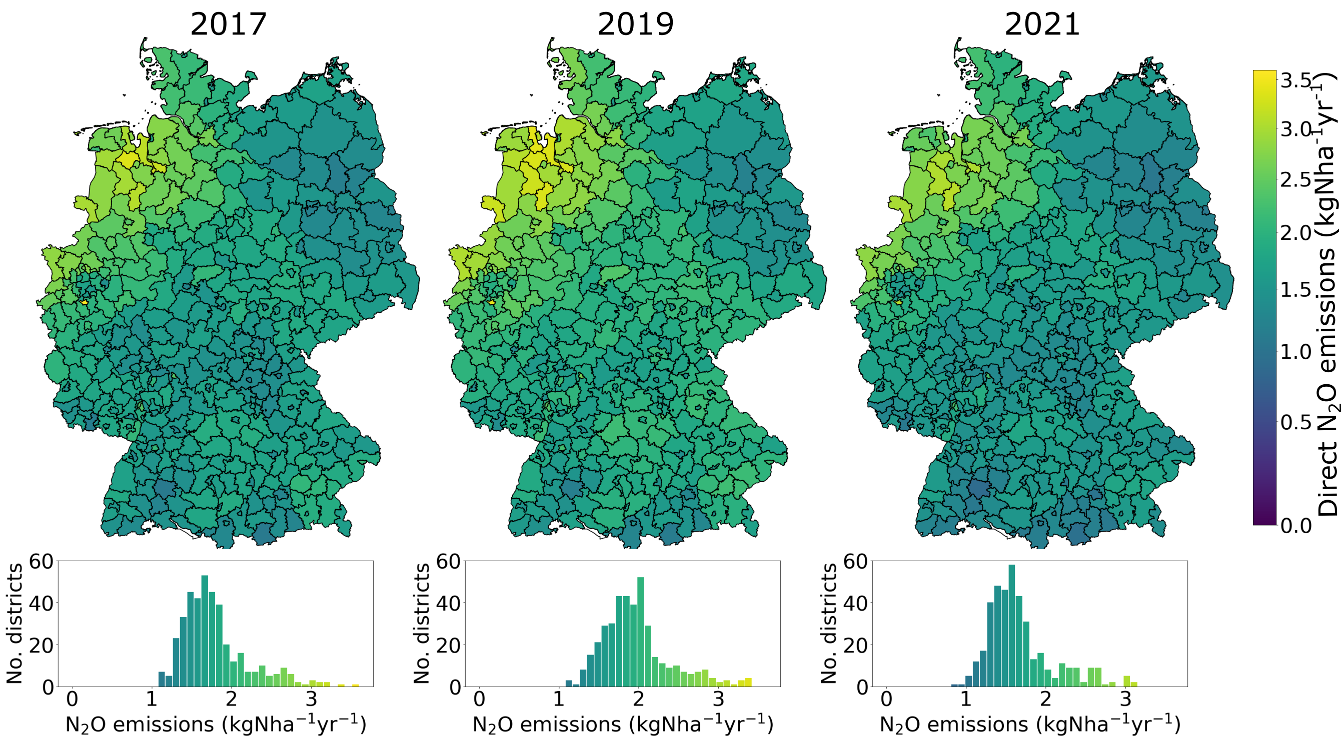

Figure 3: Direct N_2O emissions from mineral soils mapped across 403 administrative districts for the years 2017, 2019 and 2021. (Top row) Spatial distribution of emission rates. (Bottom row) Frequency distribution showing the number of districts with a given emission rate.

The sub-national Tier-3 estimates for N_2O emission can also be compared to those determined using the methods of the national inventory. The most sensible point of comparison is at the climate zone scale (see Figure 4 and C1 for a definition of climate zones), since this is the scale at which fertiliser emission factors have been determined for use in the National Inventory Document (German Environment Agency, 2025; Mathivanan et al., 2021). Figure 4a shows that the two methods are in good agreement in the Continental South and Atlantic Central climate zones. In the Continental North and Atlantic North the Tier-3 method shows higher N_2O emissions.

The two methods can also be compared at the district scale, as shown in Figure 4b. Similar patterns of differences can be seen as in the comparison at the climate zone scale, with the largest differences in Northern Germany. However, the district-scale comparison shows additional structure within these climate zones. For example, in the Atlantic North climate zone the districts in the North West show higher differences than those in the South East. In the Continental South climate zone the South East corner tends to have higher emissions using the national inventory method, while the Tier 3 method shows higher emissions in Northern Bavaria and in parts of Baden-Württemberg.

https://doi.org/10.5194/egusphere-2026-4010
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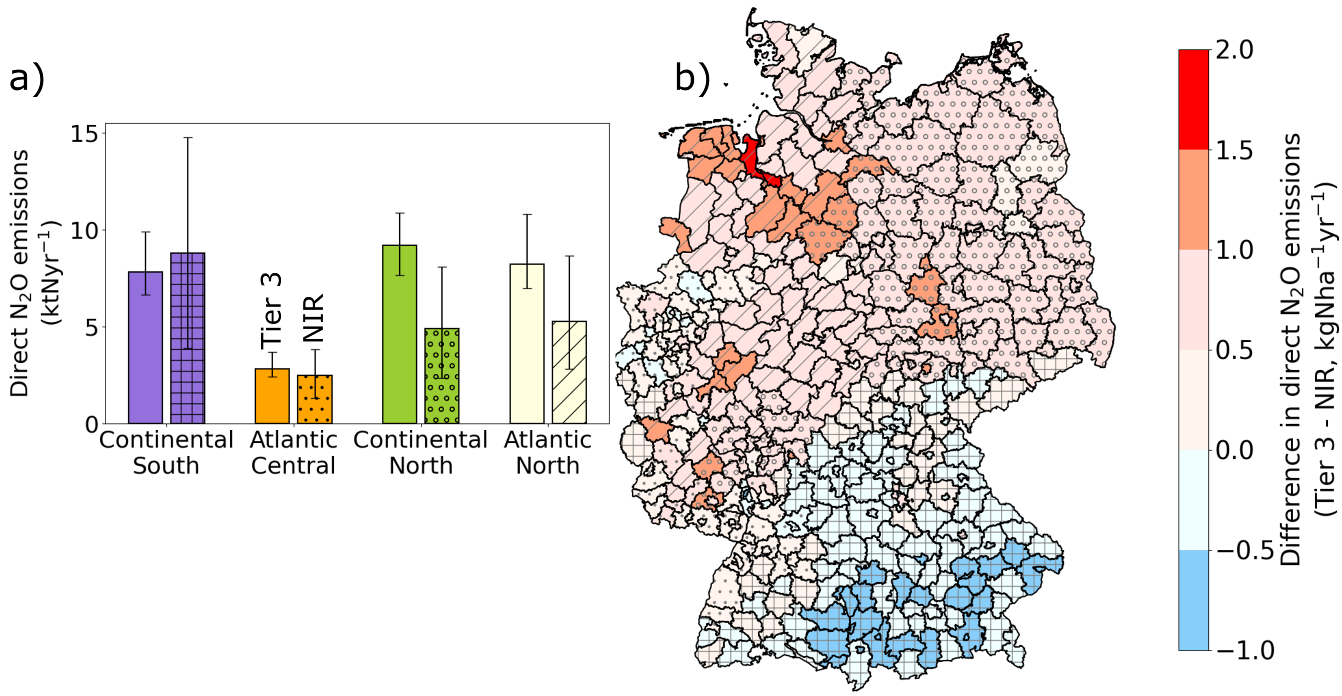

Figure 4: Comparison between sub-national direct N_2O emissions as determined by the Tier-3 method developed in this paper and the national inventory, submission 2025 (NIR). a) Direct N_2O emissions in the four main German climate zones (see Figure C1), each of which has a different fertiliser emission factor in the NIR (German Environment Agency, 2025; Mathivanan et al., 2021). Bars show average emission rates in the period 2017-2022 and whiskers the uncertainty. b) The difference in direct N_2O emission rates between the Tier 3 and NIR methods at the district scale (403 districts), averaged over the period 2017-2022. Red colours show where the Tier-3 method predicts higher emission rates and blue where the NIR predicts higher emission rates. Climate zones are shown using the same hatching as in a).

4 Discussion

Modelling framework: The Tier-3 modelling framework presented in this paper is very flexible, resulting in a number of useful features when compiling national and sub-national inventories of N_2O emissions from agricultural soils. The spatial and temporal scales can be adjusted depending on the desired output resolution, taking into account the purpose of the inventory and the resolution and quality of the input data. The spatial scale can be chosen arbitrarily by imposing an appropriate grid on the region of interest and the temporal resolution can in principle be reduced to as little as one hour, though in practice limitations on the input data will almost certainly impose a lower bound of days to weeks. For the purposes of inventory reporting to the UNFCCC a national simulation aggregated to a yearly temporal resolution is needed (German Environment Agency, 2025). At the other end of the scale, assessing the potential for the reduction of N_2O emissions via management changes requires simulations at high spatial and temporal resolution. The provision of high-resolution emission rates is also a prerequisite for the success of current efforts to improve bottom-up greenhouse-gas emission estimates by combining them with atmospheric measurements via inverse modelling, for example in the German ITMS project (ITMS

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

Germany, 2025) or the EU projects AVENGERS (Thanwerdas et al., 2025), PARIS (Walter et al., 2023) and EYE-CLIMA (EYE-CLIMA, 2026).

Within grid cells the point-sampling approach allows agricultural conditions to be represented at any desired level of detail (within the limitations of the input data). A dense sampling will precisely reproduce the different soil types, crop rotations, local climates and management practices that exist within a grid cell, while a sparser sampling will only reproduce these conditions within a tolerance set by the sampling density. The associated computational cost is related to the combination of the spatial resolution and the sampling density within grid cells, and the trade-off between this cost and the precision of the greenhouse gas emission fields is thus adjustable. Stratifying the agricultural area of each grid cell by soil, crop-type, climate and management practice followed by informed sampling from these strata could improve the representation of agricultural conditions as compared to the random sampling used here. While this would reduce the computational cost of the simulations, it would come at the price of introducing additional computational complexity in the sampling procedure itself. In particular, stratification by crop type would be complicated by the fact that crop rotations are defined for the entire simulation period. Thus, individual years are not separable, and a set of sites would have to be found that correctly reproduces yearly statistics for the whole period. Combining this with stratification of other properties is a computationally involved problem, and would likely only be tractable with a relatively wide tolerance.

The framework developed in this paper can be contrasted with other methods for producing national or international greenhouse gas inventories using process-based models. One popular method is to fix a grid-cell size and then to select a typical soil, crop rotation, local climate and agricultural management strategy within each grid cell (Carozzi et al., 2022; Del Grosso et al., 2009; Haas et al., 2022; Jägermeyr et al., 2021). If the grid cells are fixed at field-scale then this method will likely produce a very good representation of the agricultural landscape, since fields are mostly homogeneous in their agricultural conditions. However, if grid cells are considerably larger than the field scale, which is typically the case due to both computational costs and limitations of the input data, the method often fails to produce a good representation of the heterogeneous agricultural landscape. The resulting greenhouse-gas emission estimates can be misleading, as has been shown for regions of Denmark (Rahimi et al., 2024). The fixed-grid-cell method typically under-represents sub-dominant crop (e.g. legumes) and soil types, does not always produce consistent combinations of soil, crop, management and climate and gives only a superficial representation of the heterogeneous crop rotation practices within a grid cell (Rahimi et al., 2024). The point-sampling method circumvents many of these problems by performing the most accurate possible simulation at each sampled point, given the limitations of the input data. The flexibility of the method allows the sampling density to be varied so as to produce a representation of the agricultural landscape that gives the desired trade-off between precision and computational cost, allowing a good estimate of greenhouse gas emissions to be produced without simulating every field on a national scale.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

N_2O emissions in Germany: At the national scale the Tier-3 method estimates N_2O emissions that are well within the uncertainty interval of the national inventory methods (see Figure 2). Nevertheless, there are differences, with the Tier 3 method resulting in 28% higher N_2O emissions, greater interannual variability, a narrower confidence interval and a different spatial pattern, with higher emissions in Northern Germany (see Figure 4).

The difference in national N_2O emissions may be due to underestimation via the national inventory methods, overestimation by the LDNDC simulations or a combination of the two. One possible reason for an underestimation in the national inventory is related to the method used to determine fertiliser emission factors. This uses a model intercept to separate fertiliser and non-fertiliser-driven emissions, such as those due to mineralisation of soil organic matter or crop residue input. These intercepts imply non-fertiliser-driven N_2O emissions that are higher than are accounted for in the national inventory, which may imply an underestimation of emissions. Any underestimation is most likely related to the mineralisation of soil organic matter, and recent research has discussed this discrepancy in terms of the legacy effects of fertiliser application (Qian et al., 2025; Tian et al., 2024b; Vonk et al., 2022). Another potential reason for underestimation of direct N_2O emissions in the national inventory is that the fertiliser emission factors are linear, even though a non-linear response of N_2O emissions to fertiliser application rate has been documented in a number of papers (Philibert et al., 2012; Shcherbak et al., 2014; Van Groenigen et al., 2010). This may explain why the Tier-3 method shows higher N_2O emission rates in North-Western Germany, where N surpluses often exceed 100 $kgNha^{-1}yr^{-1}$ (Zinnbauer et al., 2024). On the other hand, the limitations of the N-fertiliser input data used to drive the Tier-3 method may lead to unrealistically high levels of over-fertilisation that result in an exaggerated non-linear effect and thus overestimation of national N_2O emissions. One possible reason for this is insufficient representation of manure transport between municipalities. The Tier-3 method may also overestimate N_2O emissions due to biases in the site data used to calibrate the model. However, the average yearly N_2O emission rate of the site data is considerably lower than the modelled German average (1.4 vs 1.9 $kgNha^{-1}yr^{-1}$), suggesting this is unlikely. Nevertheless, it remains possible that the process-understanding inherent in the site data results in overestimation.

The greater interannual variation in the Tier-3 method is largely due to a higher sensitivity to weather conditions. In the national inventory fertiliser-driven N_2O emissions are not weather dependent, due to insufficient measurement data to determine year-specific emission factors (Mathivanan et al., 2021). One surprise is that the Tier-3 method does not show larger interannual variation, especially in the drought year 2018, where average precipitation of 586mm was considerably lower than the 705-859mm that fell in other years in the period (Deutscher Wetterdienst, 2026). Closer investigation shows that the late summer and early autumn peak of N_2O emissions was suppressed in 2018, though it still existed. However, this was compensated by a higher than average spring peak that occurred before the start of the drought. The model does show a drought-induced reduction in crop yields in 2018, with an average N content of harvested arable crops of 133 $kgNha^{-1}yr^{-1}$, as compared to an average of 166 $kgNha^{-1}yr^{-1}$ in other years. N leaching also shows a large decrease in 2018, compensated by an increase in NH_3 emissions (see Figure D1).

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

The uncertainty associated with direct N_2O emissions is lower in the Tier 3 method as compared to the national inventory method. This is one important reason why the Tier-3 method may be preferred over emission-factor driven methods for reporting purposes, despite the increased complexity. One reason for the reduced uncertainty is that the Tier-3 method takes a larger set of drivers into account, including differences in soil, climate and agricultural management. This allows for more accurate modelling of site-level data, which translates into lower uncertainties at regional and national scale. Indirect N_2O emissions considerably increase the uncertainty of the inventory, despite being quite a small proportion of total emissions (see Figure 2). The uncertainty associated with indirect emissions is approximately the same in the Tier-3 and national inventory methods. One strategy for decreasing this uncertainty would be to estimate N_2O emissions from forests and water-bodies, where many of these indirect emissions take place.

Wider context: In the future it may be possible to replace some of the Tier-2 methods used in the German National Inventory Document with the Tier-3 method developed in this paper. This would allow approximately 70% of the N_2O emissions from agricultural soils to be estimated via a Tier-3 approach. Ongoing developments in the modelling of organic soils may also allow most of the remaining 30% to be estimated by the Tier-3 method. However, a small fraction of N_2O emissions, such as those associated with vineyards, will likely never be covered. The advantages of the Tier-3 method include reduced uncertainty and the possibility to estimate greenhouse gas emissions from agricultural soils in a unified way, as opposed to having different ways of modelling fertiliser-driven N_2O emissions, N_2O emissions driven by the mineralisation of soil organic matter and even changes in soil organic carbon stocks that result in CO_2 uptake or emission. However, it is important to note that there are a number of requirements for national inventory reporting that the Tier-3 approach does not yet fulfil. This includes extending the timescale back to 1990 and forward to the reporting year minus two (e.g. 2023 if used for the 2025 report) and improving the documentation (Calvo Buendia et al., 2019). It would also be necessary to develop a way of splitting the Tier-3 estimates of direct N_2O emissions by source, for example into those emissions arising from mineral fertiliser, manure, other organic fertilisers, crop residues and N deposition. Furthermore, it will be necessary to consider whether the additional complexity of the Tier-3 approach is desirable, both in terms of the necessity for continually-updated, high-resolution input datasets and in terms of the additional computational cost. Using the Tier-3 approach for the inventory would also require substantial additional resources and expertise in the inventory team and/or institutional arrangements that ensure integration of the approach in the operational inventory system.

The only country that has recently used a Tier-3 approach to report N_2O emissions from mineral soils is the USA, whose approach is based on the Daycent model (EPA, 2024; Ogle et al., 2020). They also use a sampling approach, based on a long-term survey of soil, crop and management information in approximately 400,000 locations, each of which has an associated larger area of which it is representative (Nusser and Goebbel, 1997; Ogle et al., 2010). This type of carefully-designed, long-term survey is considered to be the "gold standard" for producing greenhouse-gas-emission inventories (Ogle et al., 2020).

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

However, such surveys are currently unavailable in most countries and are costly to set-up and run, meaning that the approach cannot easily be replicated outside the USA. In contrast, the framework developed here can be relatively easily transferred between countries. While high-resolution and consistent datasets covering land-use, soil properties, climate and agricultural management will give the best results, the framework can still be applied using available data from already existing datasets. In terms of agricultural land-use, remote sensing products are available (and being improved continuously) for many countries and regions, for example for Africa (Xiong et al., 2017), Canada (Fisette et al., 2013) or the European Union (Ghassemi et al., 2024). Climate data is also available globally at relatively high resolution, for example ERA5-land includes hourly climate data at approximately 9km resolution (Muñoz-Sabater et al., 2021). While soil and agricultural management information are ideally available at national level, global datasets can be substituted where national data are unavailable. For example, soil properties have been mapped globally at 30 arcsecond resolution (Batjes, 2016) and crop-specific fertiliser input rates and planting dates at 0.5° resolution (Jägermeyr et al., 2021). Furthermore, LDNDC has been validated across many world regions, including in Europe (Haas et al., 2022; Molina-Herrera et al., 2016; Sifounakis et al., 2024), Africa (Fuchs et al., 2024; Rahimi et al., 2021), East Asia (Butterbach-Bahl et al., 2022; Kraus et al., 2015, 2022) and Australia (Takeda et al., 2024), making it widely applicable for determining N_2O inventories.

5 Conclusion

Accurate knowledge and reporting of greenhouse gas emissions are essential for developing targeted and effective mitigation policies. The Tier-3 method introduced in this study enhances existing Tier-2 approaches for determining N_2O emissions from agricultural soils by taking into account variations in the climate, soil type, and agricultural activity between different years and regions, allowing for reduced uncertainty and improvements in the spatial and temporal resolution of the inventory. As a result, it provides a robust foundation for evaluating mitigation strategies, such as optimizing fertiliser rates, timing, and application methods, integrating cover crops, using slow-release or nitrification inhibiting fertilisers, changing crop types and adjusting residue-management practices. Additionally, by simulating the full carbon and nitrogen cycle, the Tier 3 method offers a broad perspective on greenhouse gas mitigation, considering impacts on crop yields, nitrate leaching, ammonia volatilization, NO_x emissions and soil carbon stocks.

Appendix A: calibration and uncertainty

Model calibration: Likelihood values were assigned to each parameter set by comparing each of the 8799 measured datapoints to the simulated values and taking a product of the associated likelihoods according to,

$$L(O|\,\theta) \propto \exp\left[-\sum_{s,ty,i}\frac{m_{s,ty,i}^2}{2\,N_{s,ty}^{*}\sigma^2}\right]$$

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

where O denotes the measurement values, θ the parameter set, s labels the site, ty the treatment-year associated with the site, and i the observations associated with a particular value of s and ty. The model-data mismatch is given by $m_{s,ty,i} = \log(O_{s,ty,i}) - \log(S_{s,ty,i})$ and is the difference between the natural logs of the observed ($O_{s,ty,i}$) and simulated ($S_{s,ty,i}$) values of the N_2O emissions. The natural logs ensure an approximately normal distribution of the model-data mismatch. We assumed a diagonal form for the inverse of the variance-covariance matrix and took into account correlations at nearby times using $N^*_{s,ty}$, which denotes the average number of N_2O measurements per week (Rödenbeck, 2010). Analysis of the dataset suggest that one week is approximately the correlation time. The value σ denotes the tolerance for mismatches between the observed and simulated N_2O emission values, and we used $\sigma = 22$ in units where the N_2O emissions are measured in μg N m^{-2} hr^{-1}.

Input uncertainty was considered for synthetic and organic N fertiliser input, the soil organic matter fraction of the soil and the soil bulk density. The uncertainties associated with different spatial and temporal scales were combined via the product of multiple normal distributions. For example, the fertiliser N input for Monte Carlo run *m* in year *y* and for site *i* is given by,

$$N_{m,y,i} = N^0_{y,i}\,\mathcal{N}(1,\sigma_m^2)\,\mathcal{N}(1,\sigma_y^2)\,\mathcal{N}(1,\sigma_i^2)$$

where $N^0_{y,i}$ is the fertiliser N input for year *y* and site *i* given in the input dataset and $\mathcal{N}(1,\sigma^2)$ is a normally distributed random variable with mean 1 and standard deviation σ. A value for $\mathcal{N}(1,\sigma_m^2)$ was drawn for each Monte Carlo run and applied to all sites and years within the run, a value for $\mathcal{N}(1,\sigma_y^2)$ was drawn for each year within a Monte Carlo run and applied to all sites and a value for $\mathcal{N}(1,\sigma_i^2)$ was drawn for every site, year and Monte Carlo run. The values of the standard deviations are shown in Table A1. A similar procedure was used to construct input uncertainty for the soil properties, with the difference being that soil properties are used to initialise the model, and therefore it is not necessary to consider temporal uncertainties.

Input data	$\boldsymbol{\sigma_m}$	$\boldsymbol{\sigma_y}$	$\boldsymbol{\sigma_i}$
Synthetic fertiliser N	0.001	0.025	0.1
Organic fertiliser N	0.025	0.025	0.1
Soil organic matter fraction	0.025		0.1
Soil bulk density	0.025		0.1

Table A1: Standard deviations used to add uncertainty to input parameters.

Model structure uncertainty was introduced by using a linear mixed effects model to find a relationship between observed and modelled seasonal/yearly N_2O emissions (Gurung et al., 2020, 2026; Ogle et al., 2010, 2007, 2023). Daily N_2O measurements with varying measurement frequencies (see Table D1) were converted into seasonal/yearly emissions via linear interpolation. This method gave very similar results to both a simpler scheme in which the mean N_2O emissions from the measurements

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

were multiplied by the number of days in the season/year and to the values for seasonal/yearly emissions reported in those experimental papers that reported the quantity (see references in Table D1).

The linear mixed effects model considered is,

$$\log O_{s,ty} = \beta_0(\theta) + \beta_1(\theta) \log S_{s,ty}(\theta) + \gamma_s(\theta) + \epsilon_{s,ty}(\theta)$$

where $O_{s,ty}$ denotes the observed seasonal/yearly emissions for the site s and treatment-year ty and $S_{s,ty}(\theta)$ denotes the simulated seasonal/yearly emissions for the parameter set θ. $\beta_0(\theta)$ and $\beta_1(\theta)$ are fixed effects and $\gamma_s(\theta)$ a random effect associated with the site s and they have different values for different parameter sets. $\epsilon_{s,ty}(\theta)$ is the residual of the regression fit. The natural logs ensure that the residuals are approximately normally distributed. The likelihood weighted averages of the parameters are $\beta_0 = -0.0022$, and $\beta_0 = 0.37$. Taken together, the random effects and the residuals define a normal distribution with zero mean and with a standard deviation whose likelihood weighted average is 0.74.

N2O emission rates from sites in Germany were transformed according to,

$$P_i(\theta) = A(\theta)\, S_i(\theta)^{\beta_1(\theta)},\ A(\theta) = \exp\left[\beta_0(\theta) + \mathcal{N}\left(0, \sigma^2(\theta)\right)\right]$$

where $P_i(\theta)$ is the predicted value for yearly N_2O emission from the site, $S_i(\theta)$ the simulated value, i labels the sites and $\mathcal{N}\left(0, \sigma^2(\theta)\right)$ is a normally distributed random variable with mean 0 and a parameter-set dependent standard deviation. In practice, for each Monte Carlo run, simulated site and year the predicted value was determined by drawing a random value for the normally distributed variable. The site level uncertainty associated with model structure and uncalibrated parameters was thus built into the total uncertainty, along with the input, sampling and model parameter uncertainty.

Appendix B: model input data and setup

Land use: The core land use dataset is derived from satellite imagery and distinguishes agricultural from non-agricultural land usage in every 10×10m pixel in Germany (~4×10^9 pixels of which ~2×10^9 are agricultural) for the years 2017-2022 (Blickensdörfer et al., 2022). Pixels with an agricultural land use are assigned one of 21 possible crop types. All major crops were simulated using LDNDC, including permanent grassland (42700 km^2 in 2021), winter wheat (29500 km^2), silage maize (22600 km^2), winter barley (14800 km^2), rapeseed (10800 km^2), cultivated grass (10600 km^2), winter rye (9400 km^2), sugar beet (4200 km^2), grain maize (3900 km^2), spring barley (3500 km^2), spring oats (2700 km^2), potatoes (2700 km^2), peas (1500 km^2), lupin (1000 km^2), broad beans (700 km^2), sunflowers (600 km^2) and soy (600 km^2), giving a total simulated area of 148100-151900 km^2 in the period 2017-2022. A few minor crops were not simulated that in total cover < 6% of the agricultural area, including grapevines (1100 km^2 in 2021), hops (200 km^2), orchards (300 km^2), vegetables (3400 km^2) and other agricultural areas (4100 km^2).

The land use dataset does not distinguish maize cropping systems. In order to split silage and grain maize, which are very differently managed, we use a separate dataset that records areas of crop cultivation at the district level (Duden et al., 2024).

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

This dataset distinguishes between silage and grain maize, and for each district we determine the ratio of silage to grain maize cultivation. Each sampled point within Germany that grows maize is probabilistically assigned as cultivating silage or grain maize according to the ratio of the corresponding district.

Grassland management: Satellite imagery has also been used to determine the number and dates of grass cutting events across all 10×10m pixels in Germany assigned as grassland in the land-use dataset (permanent and cultivated) (Schwieder et al., 2022). Grassland pixels are classified by number of cuts, which strongly correlates with management intensity, with either 0 cuts (4100 km^2 in 2021), 1 cut (14600 km^2), 2 cuts (19500 km^2), 3 cuts (11200 km^2), 4 cuts (3200 km^2), 5 cuts (500 km^2) or 6+ cuts (60 km^2). Cuts are performed within the LDNDC simulations at the dates given in the dataset. The timing of manure application is also tied to the cutting date (see below).

Fertiliser input rates: Fertiliser information is provided for 9649 municipalities. The fraction of the total national fertiliser input that is applied in a particular municipality has been mapped out for the target years 2014-2016 for all important fertiliser types (mineral, manure, energy-crop digestates, compost and sewage sludge) (Zinnbauer et al., 2023, 2024). Additionally, time series of total fertiliser input at the national scale have been reported (German Environment Agency, 2025). For example, in 2021 1245 ktN of mineral fertiliser, 1100 ktN of animal manure (via spreading and grazing and including imported manure), 284 ktN of energy-crop digestates, 54 ktN of compost and 12 ktN of sewage sludge were applied, giving a total of 2693 ktN. In the period 2017-2022 total N input ranged from 2566-3143 $ktNyr^{-1}$. We here assume that the distribution of fertiliser application across the municipalities has remained fixed in the target period (2012-2022 including a 5-year spin-up) and multiply the fractional values applied in each municipality by the yearly national totals to get the total N supply in each municipality for each fertiliser type in each year.

Fertiliser supply at the municipality level (summed across fertiliser types) is then split between crops (taking into account cutting intensity for grassland) in proportion to calculated N demand following a similar method to (Häußermann et al., 2020). The N demand is determined by considering the area of each crop in each municipality (via the land-use and grass-cutting datasets described above), the crop yields (reported at district level for arable crops (Duden et al., 2024) and by cut number for grass (Landwirtschaftskammer NRW) and the typical N content per tonne of yield of different crops (Landwirtschaftskammer NRW; LFL). Crop areas are used to convert N supply per crop, year and municipality to N application rates ($kgNha^{-1}yr^{-1}$). This method of calculation ensures that the total fertiliser supply on a national scale is equal to the known yearly values.

To determine which combination of fertiliser types is applied to each crop in each municipality in each year we first group fertiliser types into mineral, manure and other organic categories (energy-crop digestates, compost and sewage sludge). Mineral fertiliser is applied as a combination of urea and ammonium nitrate according to the year-specific national split between urea and non-urea fertilisers (municipality level data is not available) (German Environment Agency, 2025). Manure

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

is assigned a C:N ratio of 14.5 (intermediate between typical values for cow and pig manure (Energypedia, 2026)) while other organic fertiliser is assigned a municipality and year dependent C:N ratio that depends on the ratio between the different components, assuming C:N ratios of 6 for energy-crop digestates (Häfner et al., 2022), 25 for compost (Compost Network, 2025) and 12 for sewage sludge (Lehmphul, 2015). At the municipality level, manure is first distributed across grassland, constrained by the lower value of either the (cut-dependent) N supply or the legal limit of 170 $kgNha^{-1}yr^{-1}$ for organic fertilisation (DüV, 2025). Remaining manure is then supplied to silage maize and finally to all other arable crops, with the same upper limits. If any manure remains after fully saturating the legal limit, it is distributed first to grassland (up to the supply-limit), then silage maize and finally all other arable crops. Other organic fertiliser is applied similarly, except that silage maize is supplied before grass and the legal limits on organic fertilisation take into account the already assigned manure. Finally mineral fertiliser is distributed so as to equal the crop-dependent N supply in each municipality. The outcome of this procedure is municipality, year and crop-dependent N application rates for each fertiliser type that can be 1) summed across fertiliser types to give the already determined crop and municipality-dependent N supply values and 2) summed across crops and municipalities to give the nationally reported totals for each fertiliser type.

Fertiliser timing: No data is available for fertiliser timing in Germany, and so we assume good agricultural practice. For arable crops we link fertilisation strategies to the plant development stage. For winter cereals and rapeseed, we assume that 25% of fertiliser is applied one day before planting (typically September/October), 50% after 35% of the required growing degree days for maturity have been accumulated (~mid March) and the remaining 25% after 45% of the required growing degree days for maturity have been accumulated (~mid April). For spring cereals, sugar beet, potatoes and sunflowers 50% is applied one day before planting (~mid April) and 50% after accumulation of 35% of the growing degree days for maturity (~mid June). For maize 50% is applied one day before planting (~early May) and 50% after accumulation of 35% of the growing degree days for maturity (~end June). For legumes all fertiliser is applied one day before planting. For grass a first fertilisation event is performed on 15th March and subsequent fertilisation events occur one day after cutting with fertilisation rates split evenly across the events.

For winter crops, organic fertiliser is applied preferentially in autumn and not at all in the third fertilisation when plant cover is too high, meaning that in the case that the organic fertiliser fraction is greater than 75% the application rates are adjusted towards earlier fertilisation. For spring cereals, organic fertiliser is only applied before planting. For maize, organic fertiliser is applied preferentially before planting, but is also allowed at the second fertilisation. For grass, the first fertilisation is purely organic, assuming sufficient organic fertiliser is available. Subsequent fertilisations may also be purely organic but may also be a mix of organic and mineral fertiliser in the case that mineral fertiliser is applied.

Crop calendars: Year-specific planting and harvesting dates for major arable crops are provided on a 1×1km grid by the German weather service, based on an observational network (Kaspar et al., 2014). For crops that are not included in this dataset (potatoes, sunflowers and legumes), planting and harvesting dates are set according to a global dataset with 0.5° resolution (Jägermeyr et al., 2021). Cultivated grass is planted 5 days after the harvest of the previous crop and harvested 5 days before planting the subsequent crop, with the roots and grass stubble ploughed in. The accumulated growing degree days required by crops to reach maturity were set to be commensurate with the known planting and harvesting dates in every 1×1km grid cell, and the accumulated growing degree days required to reach intermediary plant development stages were scaled proportionately.

Soil: We use a soil map that is created using machine learning to map out the mineral soils of Germany on a 100×100m grid, based on approximately 4000 soil samples and taking into account multiple covariates (Gebauer et al., 2022; Poeplau et al., 2020; Sakhaee et al., 2022). For each grid cell sand, silt and clay contents, bulk density and N content are provided for 5 soil depths (0-10cm, 10-30cm, 30-50cm, 50-70cm and 70-100cm). Soil organic C and N stocks are also provided for the top 30cm. In order to determine soil C contents across the soil profile we assume that they follow the same depth dependence as the N contents. Fixing the C content of the top 30cm then allows the C contents of all the soil layers to be determined. Since the consistency of the depth dependent N contents and the N stock of the top 30cm is not guaranteed, we assume that the C:N contents of the top 30cm applies throughout the soil profile, and adjust the N contents accordingly.

We exclude organic soils from the process-based simulations since 1) they are not part of the soil dataset and 2) the simulation of organic soils with LDNDC is still being developed. We do this using an organic soil map of Germany to mask out the approximately 7% of pixels in the land-use dataset with an organic soil (Wittnebel et al., 2023). Crop-specific cultivated areas are adjusted accordingly.

Climate: We use climate data from the E-OBS gridded observational dataset for Europe (Cornes et al., 2018). This has a resolution of 0.1° (approximately 10km). LDNDC requires daily data for maximum, minimum and average temperature, incoming short-wave solar radiation, humidity, precipitation and wind speed.

N deposition: N deposition data has been mapped for the years 2000, 2005, 2010 and 2015-2019 on a 1×1km grid in the PINETI-4 project (Kranenburg et al., 2024). Deposition rates are split between species (NH_4^+, NO_3^-) and also between dry and wet deposition. We assume that dry deposition is split evenly across the year and that wet deposition occurs at a constant rate per mm of precipitation. For years in the period 2000-2019 that are not included in the dataset we interpolate values at the grid-cell scale. For the years 2020-22 we assume that N deposition is the same as in 2019.

Additional field management: For each simulated point the tillage practice is assigned as either conventional or reduced depending on NUTS-2 level data (38 regions across Germany) that gives the ratio between conventional and reduced tillage (Eurostat, 2024). For conventional tillage the field is tilled to 20cm depth one day before planting and then again one day after

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

harvesting. Any organic fertiliser applied before planting is thus tilled into the soil. For reduced tillage the field is tilled to 5cm depth before planting, but not after harvesting.

We assume a residue management that is crop dependent but uniform across Germany. For silage maize 80% of above ground residues are removed from the field, for cereals (wheat, barley, oats, rye) and for grain maize 50% of above-ground residues are removed and for all other crops (potatoes, sugar beet, rapeseed, legumes) 30% are removed.

We assume that all crops are rain-fed rather than being irrigated. Outdoor irrigation covered only ~5000 km^2 in Germany in 2019 (~3% of the agricultural area) (Statistisches Bundesamt, 2025).

Districts: We present results for 403 districts in Germany (NUTS-3, Landkreise), of which one is non-agricultural (fully covered by water). Districts are defined according to the Database of Global Administrative Areas (GADM) version 4.1 (GADM v4.1, 2024).

Timeframe and spin-up: We run core simulations for the 6-year period 2017-2022. Additionally, a 5-year spin up is run for the period 2012-2016. In the spin-up period the two most common crops cultivated in the core period are rotated.

Appendix C: N_2O emissions in the national inventory document

Here we explain in detail how we applied the methods of the German National Inventory Document (submission 2025) to obtain a set of N_2O emissions that is comparable to those calculated via the LDNDC model.

Fertiliser-driven emissions: In the National Inventory Report N_2O emissions are modelled as a linear function of fertiliser input, with different emission factors for organic soils and for mineral soils in four climate zones (Mathivanan et al., 2021). For mineral soils the emission factors are 0.0049 (0.0026-0.0078) kgN_2O-N kgN^{-1} in the Atlantic North region, 0.0039 (0.0017-0.0066) kgN_2O-N kgN^{-1} in the Continental North region, 0.0072 (0.0037-0.0108) kgN_2O-N kgN^{-1} in the Atlantic Central region and 0.0088 (0.0038-0.0143) kgN_2O-N kgN^{-1} in the Continental South region, as shown in Figure C1. These emission factors integrate over soil types, local climate variations, types of N input and all other agricultural management practices. For organic soils the national emission factor is 0.0101 (0.0039-0.0165) kgN_2O-N kgN^{-1}. These emission factors were applied to the same fertiliser N input dataset as used for the LDNDC simulations.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

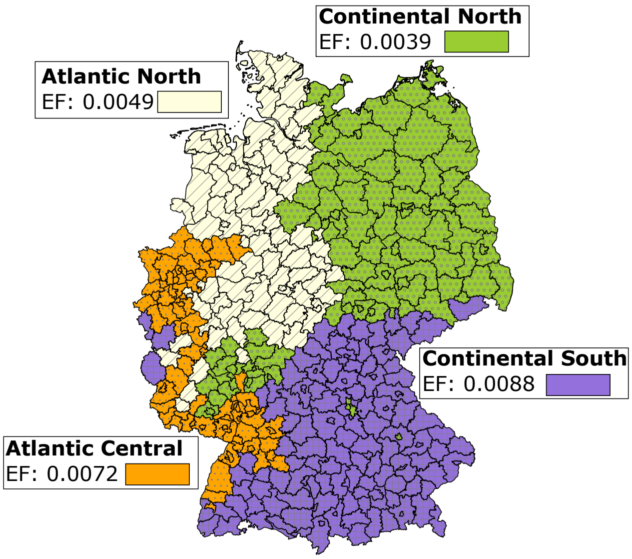

Figure C1: Emission factors (EF, $kgN_2O\text{-}N\ kgN^{-1}$) for mineral soils used as part of the Tier-2 methodology for estimating N_2O emissions (Mathivanan et al., 2021). Germany is split into 4 climate zones (Metzger et al., 2005) and these have been mapped onto administrative districts. For districts that are split between multiple climate zones, the largest climate zone by area has been selected.

Grazing: N_2O emissions from urine and dung deposited during grazing are estimated using the IPCC Tier-1 emission factors (Calvo Buendia et al., 2019). These are 0.006 (0.0-0.027) $kgN_2O\text{-}N\ kgN^{-1}$ for cattle, poultry and pigs and 0.003 (0.0-0.01) $kgN_2O\text{-}N\ kgN^{-1}$ for sheep and goats. Taking into account the numbers of grazing animals in Germany results in a national emission factor of 0.0054 (0.0-0.024) $kgN_2O\text{-}N\ kgN^{-1}$ (Vos, 2025). These were applied to the portion of N from grazing modelled by LDNDC.

Crop residues decomposition: Above and below-ground crop-residue production and N contents are estimated from crop yield data via crop-specific, tabulated values for yield-to-residue ratios, dry-matter fractions, N contents and, for grass, mowing and renewal frequency (Vos, 2025). For above-ground crop residues we assume the same fraction of crop residue removal as in the LDNDC simulations. All below-ground crop residues are assumed to remain on the field. N_2O emissions are determined from crop residue N input using the same emission factors as for fertiliser N inputs (Mathivanan et al., 2021).

Mineralisation of mineral soils: N_2O emissions due to the mineralisation of mineral soils are taken directly from the National Inventory Report. For consistency with the National Inventory Report we additionally take into account soil mineralisation due to grassland to cropland conversion. All pixels in the land-use dataset that cultivate grassland for at least 1 year in the 2017-2022 period are assumed to rotate between grass and cropland. For the years in which crops are cultivated in these pixels an N_2O emission factor of 0.55 $kgNha^{-1}yr^{-1}$ is applied (German Environment Agency, 2025).

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

Indirect N_2O emissions: For nitrate leaching a set of factors have been determined on a national scale and yearly basis that relate N leaching to the input of N fertiliser and crop residues (German Environment Agency, 2025). For the years 2017-2022 these are 0.09 , 0.11, 0.09, 0.09, 0.08 and 0.08 kgN kgN^{-1}, with an uncertainty of -100% on the lower side and +200% on the upper side. For NH_3 and NO volatilisation a similar set of percentages have been determined, but split into mineral and organic fertilisers (crop residues are assumed not to contribute to ammonia volatilisation). In the period 2017-2022 these are 0.085, 0.082, 0.079, 0.060, 0.061 and 0.061 kgN kgN^{-1} for mineral fertilisers and 0.128, 0.131, 0.127, 0.125, 0.123 and 0.125 kgN kgN^{-1} for organic fertilisers, and N volatilisation rates are subject to uncertainties of -25% on the lower side and 25% on the upper side. The IPCC estimates N_2O emission factors of 0.011 (0.0-0.02) kgN_2O-N kgN^{-1} for leached N and 0.014 (0.011-0.017) kgN_2O-N kgN^{-1} for volatilised N (Calvo Buendia et al., 2019). These factors were applied to the same fertiliser input dataset as used in the LDNDC simulations.

Appendix D: Additional figures and tables

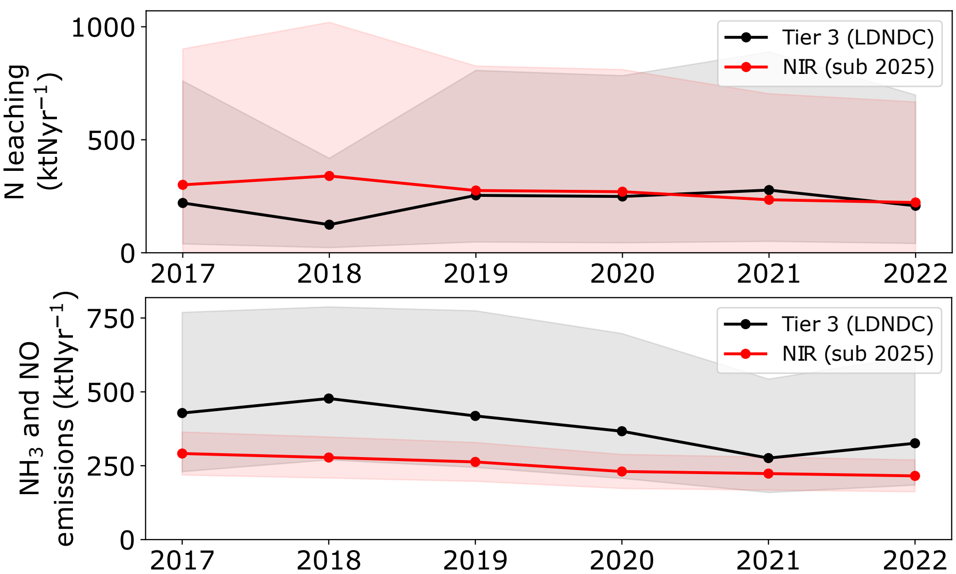

Figure D1: Comparison of N loss pathways as estimated by the Tier 3 method (black, LDNDC) and the National Inventory Report (red, NIR). (Top panel) Comparison of N leaching out of the rooting zone. (Bottom panel) Comparison of NH_3 and NO emissions. The shaded regions show the associated uncertainty intervals.

Site name and reference	Treatment notes	Year	Crop	N fertilisation rate ($kgNha^{-1}$)	Full year / growing season	No. of measurements

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

Gebesee (Lehuger et al., 2011)		2007-8	Winter wheat	355	Full Year	282
Giessen (Khan et al., 2025)	Conventional	2021	Maize	163	Growing season	190
	Conventional	2022	Rye grass	148	Growing season	116
	Organic	2021	Maize	163	Growing season	190
	Organic	2022	Rye grass	148	Growing season	110
Göttingen (Eckei et al., 2025)		2021	Sugar Beet	100	Growing season	30
		2021	Winter wheat	210	Growing season	35
Hohenheim site 1 (Guzman-Bustamante et al., 2019)	Unfertilised	2011-12	Winter wheat	0	Full Year	59
	Unfertilised	2012-13	Winter wheat	0	Full Year	55
	Low fertilisation	2011-12	Winter wheat	120	Full Year	59
	Low fertilisation	2012-13	Winter wheat	120	Full Year	55
	Conventional fertilisation	2011-12	Winter wheat	180	Full Year	59
	Conventional fertilisation	2012-13	Winter wheat	180	Full Year	55

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

	High fertilisation	2011-12	Winter wheat	240	Full Year	59
	High fertilisation	2012-13	Winter wheat	240	Full Year	55
Hohenheim site 2 (Guzman-Bustamante et al., 2022)	Unfertilised	2012-13	Winter wheat	0	Full Year	56
	Ammonium sulphate nitrate (ASN)	2012-13	Winter wheat	180	Full Year	56
	Calcium ammonium nitrate (CAN)	2012-13	Winter wheat	180	Full Year	56
	ASN-CAN-CAN split fertilisation	2012-13	Winter wheat	180	Full Year	56
Paulinenaue (Bell et al., 2012)		2008	Grain maize	122	Growing season	17
		2009	Grain maize	122	Growing season	14
Reinshof (Wang et al., 2021)	Unfertilised	2016-17	Winter wheat	0	Full Year	59
	Unfertilised	2017-18	Winter wheat	0	Full Year	69
	CAN	2016-17	Winter wheat	180	Full Year	59
	CAN	2017-18	Winter wheat	180	Full Year	69

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

	Urea	2016-17	Winter wheat	180	Full Year	59
	Urea	2017-18	Winter wheat	180	Full Year	69
	Unfertilised	2017-18	Winter rapeseed	0	Full Year	68
	CAN	2017-18	Winter rapeseed	180	Full Year	68
	Urea	2017-18	Winter rapeseed	180	Full Year	68
Renningen (Weller et al., 2019)	Unfertilised	2012	Silage maize	0	Full Year	252
	Unfertilised	2012	Silage maize	0	Full Year	304
	Urea	2013	Silage maize	177	Full Year	252
	Urea	2013	Silage maize	148	Full Year	304
Foulum (Pugesgaard et al., 2017) (Denmark)		2008-9	Spring barley	130	Full Year	20
		2008-9	Faba beans	0	Full Year	20
		2008-9	Winter wheat	165	Full Year	28
		2008-9	Potatoes	140	Full Year	24
Grignon (Loubet et al., 2011) (France)		2007	Winter barley	110	Full Year	253
		2008	Silage maize	136	Full Year	267

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

		2009	Winter wheat	78	Full Year	293
Fendt (Kiese et al., 2018)	Extensive	2014	Permanent grass	39	Full Year	302
	Extensive	2015	Permanent grass	49	Full Year	320
	Extensive	2016	Permanent grass	96	Full Year	292
	Extensive	2017	Permanent grass	88	Full Year	287
	Extensive	2018	Permanent grass	105	Full Year	269
	Intensive	2019	Permanent grass	182	Full Year	276
	Intensive	2020	Permanent grass	182	Full Year	339
	Intensive	2014	Permanent grass	206	Full Year	293
	Intensive	2015	Permanent grass	186	Full Year	314
	Intensive	2016	Permanent grass	234	Full Year	288
	Intensive	2017	Permanent grass	194	Full Year	281
	Intensive	2018	Permanent grass	182	Full Year	306
	Intensive	2019	Permanent grass	182	Full Year	262
	Intensive	2020	Permanent grass	182	Full Year	334
Graswang (Kiese et al., 2018)	Intensive	2012	Permanent grass	248	Full Year	130

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

	Intensive	2013	Permanent grass	300	Full Year	115
	Intensive	2014	Permanent grass	206	Full Year	122

640 **Table D1:** Experimental sites used to calibrate N_2O emissions in LandscapeDNDC.

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

Parameter Name	Parameter range	Description
F_SANVF_1	0.8-4.0	Relates soil anaerobic volume fraction to oxygen partial pressure
F_SANVF_2	6-10	Relates soil anaerobic volume fraction to oxygen partial pressure
KMM_C_DENIT	0.00001-0.01	Dependence of denitrifier growth on carbon availability
KMM_N_DENIT	0.0001-0.01	Dependence of denitrifier growth on nitrogen availability
F_DENIT_N2_1	0-1	Influences fraction of nitrite that is denitrified to N_2
F_DENIT_N2_2	0-1	Influences fraction of nitrite that is denitrified to N_2
F_DENIT_NO	1-20	Influences fraction of nitrite that is denitrified to NO
F_NIT_FRAC_MIC	0-1	Modifies active fraction of nitrifiers

https://doi.org/10.5194/egusphere-2026-4010
Preprint. Discussion started: 16 July 2026

KMM_NH4_NIT	0.0001-0.01	Michaelis-Menten factor linking the nitrification rate to NH_4^+ availability
KMM_O2_NIT	0.0001-0.01	Michaelis-Menten factor linking the nitrification rate to O_2 availability
KF_NIT_NO_N2O	0.001-0.12	Influences the production of NO and N_2O during nitrification
F_DECOMP_T_EXP_1	0.5-5	Dependence of organic matter decomposition rate on temperature
F_DECOMP_CLAY_2	0-10	Dependence of organic matter decomposition rate on clay content
KR_DC_HUM2	0.00005-0.003	Decay rate of old humus with high CN ratio
KR_DC_HUM3	0.000001-0.000125	Decay rate of old humus with low CN ratio

Table D2: LandscapeDNDC parameters used in the calibration of N_2O emission rates. Parameters are chosen that influence the soil anaerobic volume fraction, the denitrification and nitrification processes and the decomposition of soil organic matter.

Code and data availability

Data and codes will be made available in a public repository before publication.

Author contributions

The work was conceived by ASm, HI, CS and RK. HI and JA acquired and curated input data. ASa created a soil dataset. DK and EH developed and maintained the LDNDC model. ASm designed the methodology with help from KF, LM and CV. The investigation was performed by ASm. The project was administered by HI and supervised by CS, RK and RF. ASm wrote the manuscript with reviewing and editing from HI, CS, RK, RF, CV and JA.

Competing interests

The authors report there are no competing interests to declare.

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