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LETTER

Denitrification in biogeochemical models—challenges and advances in simulating N_2 and N_2O emission in agricultural systems

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Abstract

Denitrification represents a major nitrogen (N) loss pathway in agriculture, reducing plant N uptake, lowering crop N use efficiency, while emitting the potent greenhouse gas nitrous oxide (N_2O). However, due to methodological challenges, field measurements of N_2 emissions remain rare, leaving denitrification losses poorly characterised across most cropping systems and comprehensive N budgets lacking. This constrains parameterization and validation of biogeochemical models, impeding efforts to forecast denitrification losses under changing conditions and design effective mitigation strategies. This study (i) reviewed the current literature on field-based N_2 measurements, (ii) tested the ability of five different models to accurately simulate denitrification losses, and (iii) simulated denitrification losses from agricultural soils in Germany using gridded and point-based modelling frameworks. Results show that field studies suitable for model calibration remain scarce and mostly limited to temperate systems. Simulated cumulative N_2 emissions varied widely between models, ranging from 0.89 to 6.07 kg N ha^{-1}, far below the observed N_2 emissions of 21 ± 3 kg N ha^{-1}. The ratio of N_2O to ($N_2O + N_2$) emitted (R_{N_2O}), a key determinant of the climate impact of denitrification, was not only strongly overestimated by all models but also exhibited considerable variations, ranging from 0.056 to 0.707, compared to the measured ratio of 0.006. Models also failed to capture expected responses of to environmental drivers. For Germany, simulated average N_2 emissions from agricultural soils ranged from 1.7 to 14.5 kg N $ha^{-1}yr^{-1}$, with corresponding R_{N_2O} ratios ranging from 0.18 to 0.59. Spatial patterns of emissions also differed significantly across modelling frameworks, reflecting large structural uncertainties. These findings highlight that both N_2 emissions and R_{N_2O} ratios remain poorly represented in current models, severely limiting our ability to establish reliable N budgets and develop targeted N management strategies. Coordinated advancements in field-based measurements and modelling are urgently needed to improve the representation of denitrification in biogeochemical models.

1. Introduction

Denitrification, the microbial reduction of nitrate (NO_3^-) and nitrite (NO_2^-) to gaseous emissions of nitric oxide (NO), nitrous oxide (N_2O) and dinitrogen (N_2), represents a major pathway for nitrogen (N) loss from terrestrial ecosystems. It plays a central role in regulating the size and fate of reactive nitrogen (N_r) pools in the environment and the majority of anthropogenic N_r created each year is ultimately returned to the atmosphere as inert N_2 by terrestrial denitrification processes (Scheer *et al* 2020).

In fertilised agricultural systems 5%–30% of applied N fertiliser is assumed to be lost through denitrification (IPCC 2019), reducing plant N uptake and lowering crop N use efficiency. These N losses create significant environmental concerns; particularly due to the emissions of N_2O, which is not only a potent greenhouse gas with a global warming potential 273 times greater than CO_2 (IPCC 2021), but is also the primary contributor to stratospheric ozone depletion (Ravishankara *et al* 2009, Davidson *et al* 2014).

While significant progress in analytical techniques in the last decade have improved our process understanding at the microscale (Kleineidam *et al* 2025), data on N_2 emissions at field-relevant scales are still largely missing, hence limiting the ability to reliably upscale denitrification dynamics to larger scales (Robertson 2023). Consequently, as the anticipated largest N flux from denitrification, emissions of N_2 are a major source of uncertainty in agroecosystem N budgets. Since no method currently exists to directly quantify N_2 emissions at larger spatial scales, upscaling efforts must rely on functional relationships of measurable quantities. In this context, biogeochemical process models that operate at the field or larger scale offer a powerful tool, as they typically provide a coherent representation of the entire N cycle including all kind of ecosystem N fluxes such as storage, vegetation exchange, leaching and gaseous losses. However, the representation of denitrification processes in these models is often derived from incubations or step-tank experiments that relied on the problematic acetylene inhibition technique (AIT) (Leffelaar *et al* 1988, Parton *et al* 1996, Del Grosso *et al* 2000). Moreover, the general lack of experimental data on denitrification-related metabolic rates, particularly N_2 production, makes thorough calibration and validation of denitrification rates in these models difficult. As a consequence, N_2 fluxes are frequently neglected in model applications, leading to large variability in process formulations and parameterizations, with simulated N_2 emissions differing by an order of magnitude or more across models (Fuchs *et al* 2020, Grosz *et al* 2023). Particularly, the ratio of N_2O to ($N_2O + N_2$) emitted (R_{N_2O}), a key determinant of the climate impact of denitrification, is still poorly constrained in most models. These uncertainties restrict our capacity to predict denitrification losses in the context of changing environmental conditions, as well as our ability to develop sustainable N management strategies for agriculture.

This study (i) critically summarizes the latest research findings of denitrification losses and their control under field conditions, (ii) evaluates the ability of different process-based models to simulate N_2 and N_2O emissions at site and landscape scales, and (iii) examines how denitrification processes are currently represented in these models. By identifying knowledge gaps and proposing improvements, this study aims to enhance the predictive capacity of denitrification models to support evidence-based policy and sustainable N management.

2. Material and methods

2.1. Literature review of field-based measurements of denitrification

We conducted a literature review using the search terms 'denitrification', 'N_2', and 'agriculture' on ISI Web of Science and Google Scholar to find field based N_2 measurements. Relevant publications had to meet the following criteria: They had to report measured N_2 fluxes using either the ^{15}N gas flux method or the He/O_2 or Ar/O_2 incubation method. Studies using the AIT were excluded due to the well documented problems associated with this method (Bollmann *et al* 1997, Groffman *et al* 2006). Studies had to include a minimum of 7 measurements days directly in the field or under field-like conditions and present either cumulative results for each treatment or results in a way that enabled cumulative fluxes to be calculated over the experimental period. Laboratory studies using intact plant-soil systems where the plants were in the dark during gas flux measurement were also accepted if the denitrification product stoichiometry obtained was used to derive field N_2 fluxes in combination with high resolution *in situ* N_2O flux measurements. To supplement the database, we also screened the reference lists of all relevant publications. From the selected studies, we extracted N_2 and N_2O fluxes as well as the R_{N_2O} ratio. We used a Welch's t-test to compare group means for the following variables: land use type (arable or grassland), fertiliser type (mineral or organic), and measurement technique (He/O_2 versus ^{15}N tracer). The target variables were N_2, N_2O, emission factors (N emissions as a percentage of the fertiliser N inputs) for N_2 (EF_{N2}) and N_2O (EF_{N2O}), and total denitrification.

2.2. Site & regional simulations

2.2.1. Simulations of site-scale denitrification losses

Five biogeochemical models were tested based on their ability to accurately simulate denitrification losses from a well-defined *in-situ* lysimeter experiment (Yankelzon *et al* 2025a). These models included

LandscapeDNDC (LDNDC) (Haas *et al* 2013), DNDC-Can (Smith *et al* 2020), MONICA (Nendel 2014), APSIM (Holzworth *et al* 2014), and DayCent (Parton *et al* 1998). The five models estimate N_2 and N_2O emissions in different ways (references to the applied model version are provided in the supplementary material).

The models LDNDC and DNDC-Can use a process-oriented Michaelis–Menten kinetics approach to describe nitrification and denitrification processes and implement the concept of aerobic and anaerobic soil volumes driven by O_2 concentration. Nitrifying and denitrifying models are explicitly modelled. In contrast, DayCent, MONICA and APSIM apply empirically derived relationships to describe N_2O and N_2 production rates of nitrification and denitrification using sets of soil physical and chemical parameters without linking those rates to explicitly modelled O_2 concentrations and nitrifying/denitrifying microbial communities.

Each model used the same input data including information on initial soil properties, daily weather variables and agricultural management. Initial soil properties provided for each soil horizon included bulk density, pH, soil texture (i.e. clay, silt and sand content), and organic carbon (C) and N content. The daily weather data included maximum and minimum temperature (°C), precipitation (mm), relative humidity (%), global radiation (W m^{-2}) and wind speed (m s^{-1}).

The rationale behind the selection of this data for model testing was the comprehensive set of relevant variables that were measured: The experiment provided measurements of all major N fluxes, including plant N uptake, NO_3^- leaching and ammonia (NH_3), N_2 and N_2O emissions, during one winter wheat growing season (Yankelzon *et al* 2025a).

2.2.2. Simulations of regional denitrification losses

Two modelling approaches were employed to estimate denitrification losses from agricultural soils in Germany. LDNDC used a gridded framework with high-resolution input data on crop types (10 × 10 m), soil properties (100 × 100 m), fertiliser inputs across ∼10 000 municipalities, planting/harvesting dates, and N deposition (1 × 1 km) for the period 2017–2022 (Smerald *et al* 2025). For each administrative district, 100 representative fields were simulated. District-level denitrification was calculated by averaging the fields with equal weighting. National N_2 and N_2O emissions were derived from area-weighted grid cell averages.

MONICA and DNDC-Can used a point data approach based on 1236 cropland sites from the German Agricultural Soil Inventory (Poeplau *et al* 2020), with simulations covering 2007–2010. Total denitrification losses at the district level were then determined by averaging over the simulated sites in each district. For each of these sites, measured soil properties (soil organic carbon, C:N ratio, texture, pH, bulk density) were available up to a depth of 1 m. Management data were collected via farmer questionnaires for a period of 10 years. Timings of management operations were derived based on phenological stages of agricultural crops (Ouattara *et al* 2025). Weather data were taken from adjacent weather stations of the German Weather Service station network (DWD 2024). Simulations were preceded by spin-up runs of 3 years.

3. Results and discussion

3.1. Field based measurements of denitrification

A comprehensive review of the literature identified 25 relevant publications on N_2 fluxes under field or field-like conditions (table 1, and SI), comprising 99 observations linked to specific site-treatment combinations. This number is substantially lower than that of a recent meta-analysis by Pan *et al* (2022a), which included studies using the AIT. In contrast, our strict inclusion criteria excluded AIT-based studies and those lacking direct measurements under field or field-like conditions, demonstrating the continued scarcity of field data suitable for model calibration.

These studies, published between 1978 and 2025, show that despite decades of research, the number of studies suitable for calibrating biogeochemical models with realistic field data on denitrification losses is still extremely limited. Moreover, the data show a clear geographical and climatic bias: most experiments were conducted in temperate systems, with only four in subtropical environments, one in an irrigated semi-arid system and one in a tropical sugarcane system (figure 1).

The majority of observations (80) were conducted on arable land, while two observations were made in a paddy rice system and 17 in grasslands. No significant differences in denitrification rates were found between arable and grassland systems ($p > 0.05$), nor did fertiliser type significantly affect denitrification or the average R_{N_2O} ratio ($p > 0.05$). However, there was a tendency toward higher R_{N_2O} with mineral fertiliser compared to organic fertiliser ($p = 0.07$), a trend that warrants further study.

Both helium/oxygen (He/O_2) and ^{15}N tracer techniques yielded similar mean N_2 and N_2O fluxes, emission factors, and R_{N_2O} values, indicating both methods are suitable for quantifying N_2 emissions at field scale (Friedl *et al* 2020). Measured cumulative N_2 fluxes ranged from 0 to 209 kg N ha^{-1}, with a mean of 20 kg N ha^{-1}. However, the reported denitrification losses were measured over highly variable observation periods (from two weeks to a full year) and across a wide range of fertiliser application rates (0–800 kg N ha^{-1} of mineral and organic fertiliser N combined), making direct comparisons of absolute

Table 1. Summary of available field data with N_2 measurements. N_2O:(N_2 + N_2O) ratios (RN_2O), Emission factors (EFs[a]) for N_2 (EFN_2) and N_2O (EFN_2O) as well as cumulative N_2O and N_2 emissions over the duration of the experiment from 99 observations (site*treatment combinations) published in 25 publications between 1978 to 2025.

Study type	*n*	R_{N_2O}	$EF_{N_2O+N_2}$ (%)	EF_{N2O} (%)	EF_{N2} (%)	N_2O (kg Nha^{-1})	N_2 (kg Nha^{-1})	Total (kg Nha^{-1}yr^{-1})
Arable	74	0.16 (±0.02)	8.5 (±1.2)	1.3 (± 0.3)	7.3 (±1.2)	2.3 (±0.5)	15.8 (±3.2)	18.2 (±3.4)
Grassland	23	0.09 (±0.02)	13.1 (±1.8)	1.2 (± 0.3)	11.9 (±1.7)	2.7 (±0.7)	31.7 (±9.2)	34.3 (±9.5)
Paddy rice	2	0.01 (±0.00)	22.8 (±1.6)	0.2 (±0.0)	22.8 (±1.6)	0.3 (±0.1)	50.2 (±3.5)	50.6 (±3.6)
Mineral fertiliser	40	0.19 (±0.04)	9.0 (±2.0)	0.8 (±0.1)	8.3 (±2.0)	1.9 (±0.3)	18.7 (±5.6)	20.6 (±5.9)
Organic fertiliser	57	0.11 (±0.02)	10.0 (±1.0)	1.5 (±0.5)	8.5 (±1.0)	2.8 (±0.6)	20.2 (±4.1)	23.0 (±4.3)
^{15}N gas flux	80	0.14 (±0.02)	9.6 (±1.1)	1.2 (±0.3)	8.4 (±1.1)	2.3 (±0.5)	19.7 (±3.9)	22.0 (±4.1)
He/O_2	17	0.13 (±0.03)	9.8 (±2.2)	1.3 (±0.3)	8.5 (±2.2)	3.0 (±0.7)	18.9 (±5.5)	21.9 (±5.6)
All upland soils	97	0.14 (±0.02)	9.7 (±1.1)	1.2 (±0.3)	8.4 (±1.0)	2.4 (±0.4)	19.6 (±3.3)	22.0 (±3.5)
All data	99	0.14 (±0.02)	9.9 (±1.2)	1.2 (±0.3)	8.7 (±1.0)	2.4 (±0.4)	20.2 (±0.3)	22.6 (±3.4)

[a] EFs are defined as N emissions as a percentage of the fertiliser N inputs.

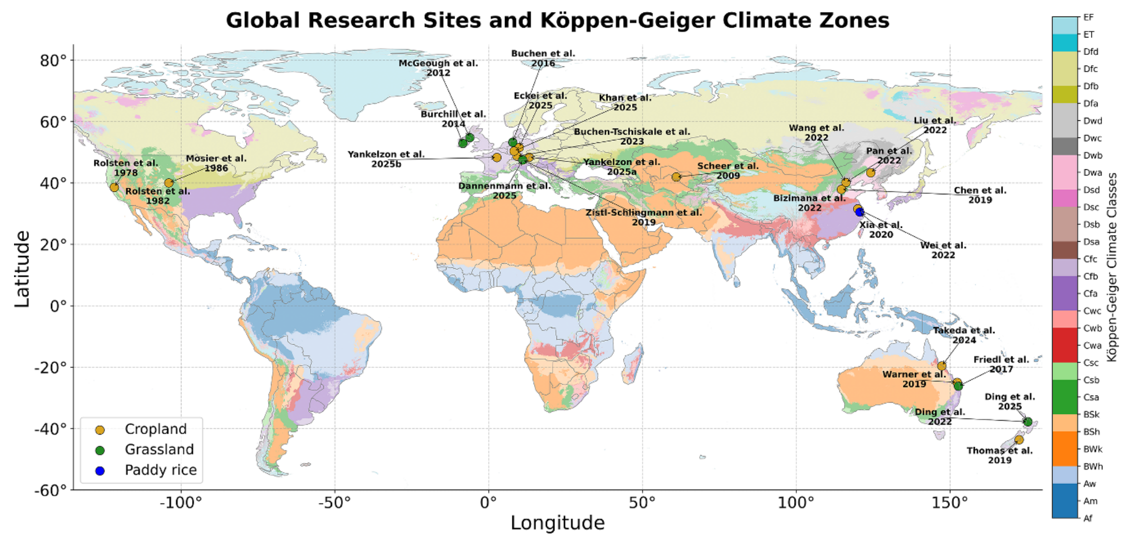

Figure 1. Spatial distribution of the N_2 experiments at arable, grassland and paddy rice fields corresponding to the studies collected in the literature review.

values challenging. The average R_{N_2O} was 14%, which is consistent with recent findings—a meta-analysis by Kleineidam *et al* (2025) reported an average R_{N_2O} of 15%, and global estimates for terrestrial denitrification by Scheer *et al* (2020) suggested 8% (with a range of 6%–11%), and 11% for agricultural soils. These values are significantly lower than those reported in previous reviews that included studies using the AIT, but it is now well established that AIT significantly overestimates R_{N_2O} and should therefore not be used to estimate field-based denitrification losses (Friedl *et al* 2020).

The mean emissions factor for N_2 emissions (EF_{N2}) was 8.7% ± 1.0% of applied N emitted as N_2, comparable to the 10.0% ± 1.5% reported by Kleinadam *et al* (2025). However, such an emission factor does not align with values estimated from global N budgets. Scheer *et al* (2020) estimated N_2 emissions from global agricultural soils at about 45 (38–55) Tg N yr^{-1}, corresponding to an EF_{N2} of 28% (24% to 34%). Moreover, Zhang *et al* (2021) estimated that more than 50% of total N inputs to croplands are lost via atmospheric emissions, leaching, and runoff, which is hard to reconcile with an EF_{N2} of 10% or lower.

One likely reason for the low EF_{N_2} values is the short duration of most field studies, which often measure N_2 emissions only over a few weeks, whereas emission factors should reflect annual losses. Additionally, subsoil denitrification—commonly excluded from surface flux measurements—can contribute substantially to total N_2 emissions, with reported rates up to 60–70 kg N ha^{-1} yr^{-1} (van Cleemput 1998). Recent evidence also shows that field surface flux measurements using the ^{15}N gas flux method can severely underestimate true denitrification rates, as a significant fraction of these gases may diffuse into the subsoil rather than being emitted at the surface (Well *et al* 2019). Furthermore, N_2 fluxes may only occur after soil drainage facilitates gas diffusion or appear late in the growing season (Ding *et al* 2022, Almaraz *et al* 2024). As a result, such fluxes may be missed if the measurement period is too short or sampling frequency too low to capture sporadic but substantial emission events.

In summary, although field-based measurements of N_2 emissions have increased and methodologies improved over the past decade, substantial data and methodological gaps persist. Denitrification losses remain poorly characterized across most global cropping systems, and comprehensive N budgets are still largely lacking. These shortcomings hinder the accurate parameterization and validation of biogeochemical models, restrict the development of effective mitigation strategies, and reduce confidence in N_2 simulations—particularly in comparison to N_2O—underscoring the urgent need for improved field-based measurements and more robust model calibration that explicitly accounts for the magnitude and dynamics of N_2 losses.

3.2. Modelling denitrification in ecosystem models

3.2.1. Site scale simulations

Denitrification associated N losses are challenging to model, as denitrification is not an isolated process chain—it is embedded within a complex network of biogeochemical interactions. These include upstream processes that produce NO_3^-, such as nitrification, as well as competing pathways for NO_3^- consumption, including microbial assimilation, plant uptake, and transport. This interdependency complicates targeted model development, comparison, and validation. To address these challenges, we assessed how five biogeochemical models represent key denitrification processes, particularly N_2 emissions and R_{N_2O}, and how well they capture the observed patterns from an *in situ* lysimeter experiment with winter wheat under fertigation (171 kg N ha^{-1} yr^{-1}).

Soil moisture is a key regulator of biogeochemical processes and is typically modelled with vertical resolution aligned to field measurements (figure 2). Its dynamics are largely governed by standard model boundary conditions (e.g. precipitation, irrigation) and consistently represented using approaches like the Richards' equation or the tipping bucket model. As a result the simulated soil moisture showed strong agreement across models. Similarly, soil temperature is primarily driven by atmospheric air temperature and handled uniformly via the heat diffusion equation (results not shown).

Regarding the metabolic switch to denitrification under anoxic conditions, soil O_2 is the direct and physiologically relevant driver. Among the models assessed, LDNDC and DNDC-Can explicitly incorporate soil O_2 as a key control on denitrification, DayCent uses respiration activity while the others rely on soil moisture. In LDNDC and DNDC-Can, the simulated O_2 is used to divide the soil into aerobic and anaerobic soil volumes. While based on the same basic concept, the implementation and interpretation of it leads to significantly different results especially during the early season (see figure 2). This discrepancy arises because the anaerobic soil volume is treated more as an expedient parameterizable functional dependency of upstream processes such as denitrification on O_2 availability rather than being evaluated against measurements directly. Although methods for measuring soil O_2 are well established, such data are often unavailable. This likely explains why biogeochemical models often use soil moisture as a proxy for anaerobic conditions. However, this can overlook critical dynamics because moisture levels do not always reflect O_2 availability. For example, microbial respiration triggered by C inputs can rapidly deplete O_2, independent of moisture levels.

Simulated cumulative N_2 emissions varied considerably between models, ranging from 0.89 to 6.07 kg N ha^{-1} yr^{-1} (table 2), well below the observed N_2 emissions of 21 ± 3 kg N ha^{-1} yr^{-1}. Nevertheless, several models reproduced the timing of N_2 peaks reasonably well, suggesting they capture denitrification dynamics but underestimate flux magnitude (figure 2). In contrast, N_2O emissions were overestimated by all models, ranging from 0.35 to 2.79 kg N ha^{-1} yr^{-1}, compared to an observed value of 0.13 kg N ha^{-1} yr^{-1} (table 2). The dynamics of N_2O emissions were captured well by some models, but the magnitude of peak emissions was in all cases overestimated (figure 2). While this overestimation was small to moderate for all models in April and May, several models simulated much higher N_2O peaks than observed during June and July. Across models, the share of N_2O production attributed to nitrification ranged from 2% (DNDC-Can) to 77% (DayCent), with the remaining 23%–98% originating from denitrification. These contrasting values again highlight fundamental conceptual differences among models and demonstrate that similar overall results may arise from different underlying process representations. However, we cannot validate these pathway contributions directly, as isotopomer measurements or ^{15}N labelling of the NO_3^- pool would be required to determine the origin of N_2O in the field (Micucci *et al* 2025). This limitation is still a major challenge in model parametrization and evaluation: while soil surface N_2O emissions are widely measured, they typically do not distinguish between nitrification- and denitrification-derived N_2O. Globally, current estimates suggest roughly equal contributions from both processes (≈50:50), but this ratio can vary considerably depending on site-specific conditions and ecosystem types (Han *et al* 2024).

A comparison of simulated and measured R_{N_2O} ratios reveals a substantial discrepancy (table 2). Due to the high N_2 and low N_2O emissions in this trial, the observed R_{N_2O} ratio was very low (0.006). In contrast, the models simulated a higher R_{N_2O} ratio, ranging

Table 2. Observed and simulated cumulative N_2 and N_2O emissions, and N_2O:($N_2 + N_2O$) ratios (R_{N_2O}) as well as simulated N_2O production from nitrification and denitrification for the lysimeter experiment published in Yankelzon *et al* (2025a). The observation period for which N_2 was measured was 21.4 to 02.7.2021, thus all quantitative comparisons refer this this period.

Model	N_2 emission (kg N ha^{-1} yr^{-1})	N_2O emission (kg N ha^{-1} yr^{-1})	N_2O nitrification (kg N ha^{-1} yr^{-1})	N_2O denitrification (kg N ha^{-1} yr^{-1})	R_{N_2O} (-)
Observed	21.00	0.134	NA	NA	0.005
LDNDC	5.776	0.345	0.055 (16%)	0.289 (84%)	0.056
DNDC-Can	3.048	2.075	0.052 (2%)	2.024 (98%)	0.405
MONICA	1.153	2.785	0.382 (14%)	2.404 (86%)	0.707
DayCent	0.845	1.078	0.833 (77%)	0,245 (23%)	0.561
APSIM	6.069	0.611	0.174 (28%)	0.438 (72%)	0.092

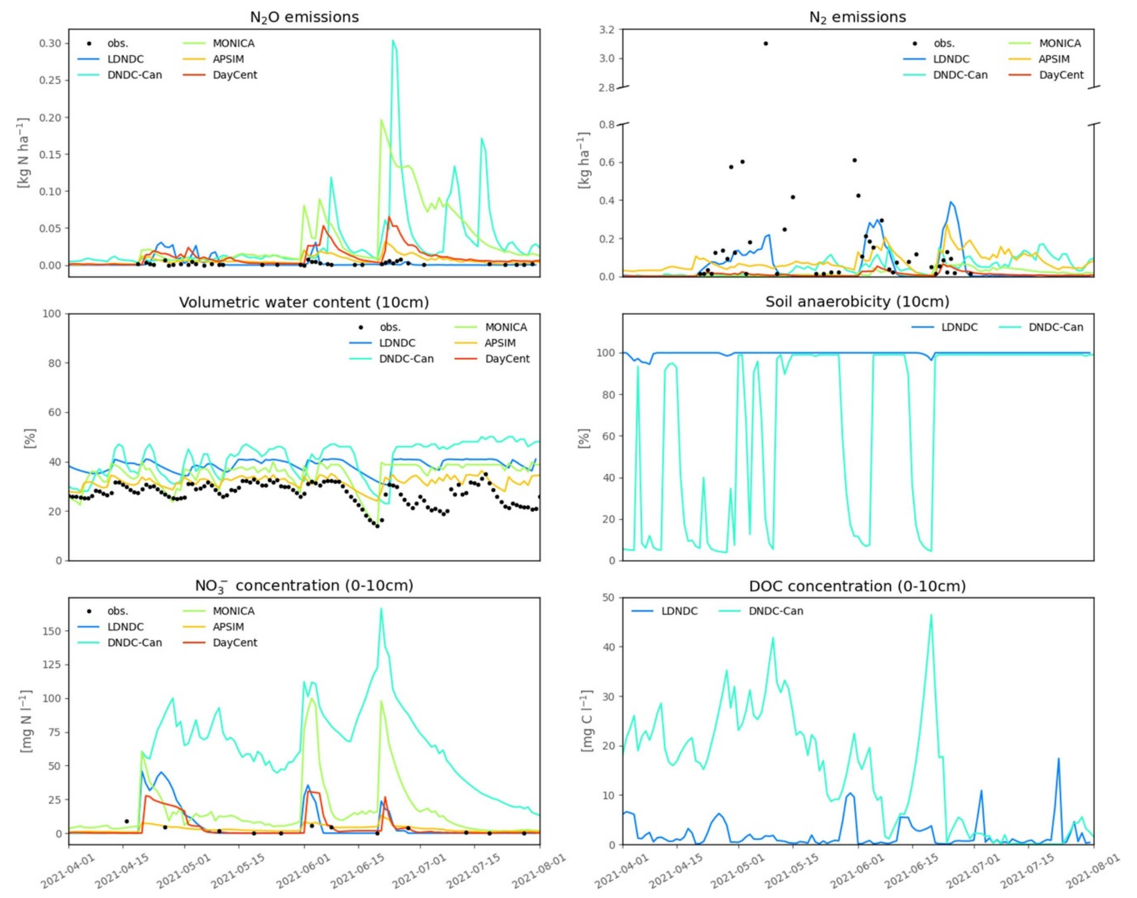

Figure 2. Comparison of N_2O and N_2 emissions and potential denitrification drivers: soil water content and anaerobicity at 10 cm depth, and NO_3^- and DOC concentrations in the 0–10 cm soil horizon. Soil anaerobicity and DOC concentrations are only simulated in the models (DNDC and DNDC-Can) and are not supported by measurements.

from 0.056 in the LDNDC simulations to 0.707 in the MONICA simulations. R_{N_2O} is sensitive to NO_3^- and C availability: high NO_3^- favours incomplete denitrification and elevated R_{N_2O} (Senbayram *et al* 2020). NO_3^- levels, in turn, are influenced by upstream N cycling processes such as mineralization, nitrification, and plant and microbial uptake, as well as by N loss pathways including NH_3 volatilization and NO_3^- leaching. Inaccurate representation of these processes may lead to poor estimates of NO_3^- concentrations and errors in denitrification dynamics and R_{N_2O} ratios. However, it is important to note that NO_3^- concentrations were measured at depth 10 cm using soil water suction cups. The fact that the models overestimated NO_3^- can partly be attributed to this sampling technique, which differed from the soil extraction method which is typically used for model testing (Djurhuus *et al* 1995). Despite large biases in simulated NO_3^-, a correlation analysis (see SI figure 1.1–1.9) showed a positive relationship between R_{N_2O} and NO_3^- across all models, consistent with the literature, underscoring NO_3^- availability as a robust driver of denitrification and R_{N_2O}.

Carbon availability is equally important, as denitrification is a heterotrophic process. Greater availability of labile C generally enhances denitrification and reduces R_{N_2O} (Weier *et al* 1993, Miller *et al* 2008). However, accurately representing C quality and accessibility in models is challenging. Most models abstract C availability using a simplified bulk pool of dissolved organic carbon (DOC). In this study, only LDNDC and DNDC-Can simulated DOC dynamics. Interestingly, R_{N_2O} emissions were lower in LDNDC despite its lower simulated DOC concentrations, suggesting that higher C availability does not necessarily directly translate into more complete denitrification, as reported in the literature. Although a linear correlation analysis revealed a positive relationship between R_{N_2O} and DOC for both DNDC and LDNDC, an additional partial dependency analysis showed that R_{N_2O} may not exhibit a consistent upward or downward trend in relation to DOC concentrations. This pattern may partly result from cross-correlations with other drivers; for example, a positive correlation between DOC and NO_3^- could mask or alter the direct effect of DOC on R_{N_2O}. Negative correlations with soil moisture and anaerobicity further complicate the interpretation, highlighting that carbon availability in the models interacts strongly with multiple environmental factors rather than acting as an independent driver.

In addition to C and N, pH is a well-known modulator of R_{N_2O} (Samad *et al* 2016). Under acidic conditions ($pH < 6$), R_{N_2O} levels tend to increase, independent of soil type (Čuhel and Šimek 2011). The experimental site's neutral pH (7.3), should favour low R_{N_2O}, across all models, again highlighting structural differences (table 2). While pH is a dynamic variable that can show significant microscale variation and influence denitrification enzyme activity, most models do not account for these microscale fluctuations. Instead, they rely on a static, site-specific pH value at initialization, and are not able to capture potential dynamic effects of pH on denitrification.

Microsite variability remains another major modelling challenge to field-scale biogeochemical modelling. Anaerobic microsites within otherwise well-aerated soil can develop due to localized high respiratory activity (Robertson 2023). These microsites are hard to represent in models regardless of whether they rely on bulk O_2 concentrations or water saturation. Schlüter *et al* (2025) proposed a novel approach using the spatial distance between organic matter and air-filled pores to simulate anaerobic conditions. While promising, this method has yet to be applied or evaluated at the field scale. Microbial denitrification pathways are highly simplified in models. Although denitrification is driven by microbial community structure and enzyme regulation, most models either simulate R_{N_2O} as an emergent property of microbial kinetics (e.g. LDNDC and DNDC-Can), or as a state variable influenced by environmental factors like pH, DOC and temperature (e.g. DayCent), thereby abstracting the underlying processes. Nevertheless, this abstraction is necessary in order to balance complexity with the availability of input parameters.

Ideally, the observed data would exhibit the expected relationships between R_{N_2O} and its environmental drivers, enabling a more robust analysis of the models. However, the scarcity of field measurements often limits such analyses. For the observational dataset, only the relationship between R_{N_2O} and soil water content could be evaluated, and no clear pattern emerged from these measurements. This lack of strong observational constraints makes it difficult to disentangle whether unexpected modelled relationships (e.g. between R_{N_2O} and C) reflect structural model errors or real environmental variability.

3.2.2. Regional simulations

We simulated N_2O and N_2 emissions for 403 administrative districts across Germany using two modelling frameworks and three process-based models (figure 3). While average national N_2O emissions were relatively consistent, substantial differences were found in the simulated N_2 emissions (table 3). For 2017–2022, LDNDC simulated an average of 14.5 kg N ha^{-1} of N_2, compared to just 1.7 kg N ha^{-1} by MONICA for 2007–2010.

A correlation analysis revealed notable differences in the main drivers of denitrification among the different models and modelling frameworks (Figure SI 2). In LDNDC, denitrification losses were primarily driven by the fertilizer N input rate. In contrast, in MONICA and DNDC-Can denitrification was mainly influenced by soil clay content, pH, and SOC, with only a minor effect of fertilizer inputs. These discrepancies highlight persistent uncertainties in regional N budgets and denitrification estimates. Some of these differences are likely attributable to the modelling frameworks themselves, as previous studies have shown that the representation of field management can introduce substantial uncertainty in regional N flow simulations (Rahimi *et al* 2024). MONICA and DNDC-Can used point-based simulations (1,236 measured sites), with each district represented by 1–25 points. With this low spatial density, the resulting N emission patterns largely reflect the variability of reported site-specific management and observed soil characteristics. In contrast, LDNDC employed a gridded approach based on national statistics and remote sensing, covering over 40 000 grid cells across Germany. Furthermore, the differing simulation periods (2007–2010 for MONICA and DNDC-Can; 2017–2022 for LDNDC) could have influenced the results. However, since climatic conditions and average fertilizer application rates were comparable between the two periods, the effect of differing simulation years on model outcomes was likely limited.

Notably, MONICA and DNDC-Can simulated much higher R_{N_2O} ratios than LDNDC, consistent with the site-level simulations (table 2). These high

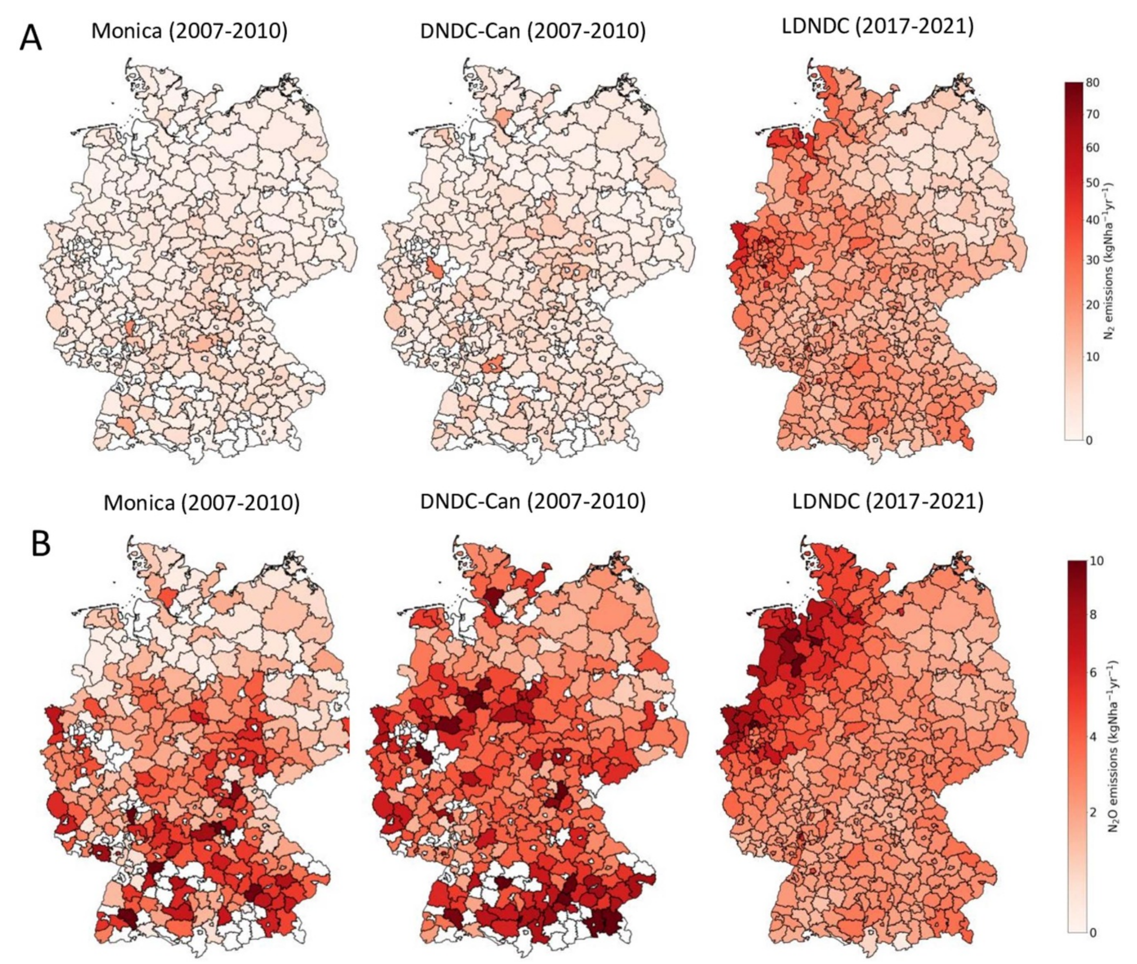

Figure 3. Simulated N_2 (A), and N_2O (B) emissions for the different administrative districts in Germany. Simulations using the MONICA and DNDC-Can models were performed for the period 2007–2010, based on point data from the German agricultural soil survey. Simulations using the LDNDC model were performed for the period 2017–2022, employing a gridded approach with high-resolution input data from the German Federal Crop Statistics. Districts with no available input data for simulation are shown in white.

Table 3. Simulated average N_2 and N_2O emissions, total N fertiliser inputs, N_2O:($N_2 + N_2O$) ratios (R_{N_2O}), and emission factors (EFs[a]) for N_2 (EF_{N2}) and N_2O (EF_{N2O}) for the different administrative districts in Germany, as well as corresponding emission factors. Simulations using the MONICA and DNDC-Can models were performed for the period 2007–2010, based on point data from the German agricultural soil survey. Simulations using the LDNDC model were performed for the period 2017–2022, employing a gridded approach with high-resolution input data from the German Federal Crop Statistics.

	MONICA (2007–2010)	DNDC-Can (2007–2010)	LDNDC (2017–2022)
N_2O emissions (kg-N ha^{-1} yr^{-1})	2.34	3.70	3.10
N_2 emissions (kg-N ha^{-1} yr^{-1})	1.69	2.57	14.50
N fertiliser input (kg-N ha^{-1}yr^{-1})	178.2	178.2	182.6
R_{N_2O}	0.58	0.59	0.18
EF_{N2O} (%)	1.31	2.08	1.70
EF_{N2} (%)	0.95	1.44	7.95

[a] EFs are defined as N emissions as a percentage of the fertiliser N inputs.

ratios conflict with values reported in the literature (table 1) and global scale denitrification estimates (Scheer *et al* 2020), thus underscoring the findings of the site simulations that these models tend to underestimate N_2 emissions. However, estimates of EF_{N2} and R_{N2O} ratios from both the data collections used in this study and global budgets also vary substantially (50%–100%) underpinning the need for a more comprehensive data base to evaluate bias and uncertainty of model estimates. The high variability across models and regions underscores the challenge of identifying denitrification hotspots and assessing regional N losses with current modelling approaches.

4. Conclusion

This study highlights major inconsistencies in how denitrification losses and R_{N_2O} are represented in biogeochemical models. While N_2O emissions were simulated relatively consistent across models, modelled N_2 emissions varied by more than an order of magnitude, reflecting structural differences in the implementation of key processes related to denitrification across models. This is exacerbated by a lack of field data on N_2 fluxes, limiting thorough calibration of these processes and validation of the results at a field level. Furthermore, the absence of detailed spatial data on land use, soil type, and agricultural management restricts our ability to generate robust N budgets at a regional level, identify emission hotspots of environmental N pollution, and design effective strategies to improve N use efficiency. Consequently, denitrification losses in the form of gaseous N_2 emissions from agricultural soils remain a major uncertainty in N budgets, particularly at field and landscape scales.

To overcome this knowledge gap, field experiments are required that not only measure N_2 emissions directly under field conditions, but also quantify the full N budget of a cropping system. Additionally, a more comprehensive evaluation of the drivers of denitrification to N_2 is needed to improve our understanding of this process and its representation in models. Recent advances in measurement techniques offer promising opportunities to develop standardized protocols to assess N_2 fluxes, helping to resolve key uncertainties in N cycling. Integrating field and lab-based experiments with advanced methods—such as ^{15}N tracing and N_2O isotopomer analysis—and ^{15}N stable isotope-based modelling (Denk *et al* 2019) offers a new way to refine biogeochemical models and provide benchmark datasets essential to reduce model uncertainty.

This will advance process-based representations of N fluxes, enabling more accurate and scalable systems-level modelling. As previously demonstrated, numerous processes that could significantly influence the results are either absent or not implemented in sufficient detail in the models. Researching and integrating these processes into the models is an important task, but the first step is to assess the current capabilities of the models. Detailed N-balance data would enable the calibration and testing of the models and reveal their shortcomings, and guide targeted model improvements.

Combining the strengths of individual models for predicting denitrification losses in different cropping systems through model intercomparison and ensembles should improve accurate estimates of denitrification and reduce associated uncertainties, thereby supporting evidence-based policy and sustainable N management.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Supplementary data 1 available at http://doi.org/10.1088/1748-9326/ae2494/data2.

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