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Modeling Denitrification: Can We Report What We Don't Know?

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Key Points:

- Biogeochemical models simulate soil denitrification through multiple pools/processes, but the N budgets reported are incomplete
- Missing (unpublished) model outputs are critical for model evaluation, model intercomparison, and model development
- Ecosystem N modelers need to support and encourage the publication of all relevant N model outputs for denitrification modeling

Supporting Information:

Supporting Information may be found in the online version of this article.

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Abstract Biogeochemical models simulate soil nitrogen (N) turnover and are often used to assess N losses through denitrification. Though models simulate a complete N budget, often only a subset of N pools/fluxes (i.e., N_2O, NO_3^-, NH_3, NO_x) are published since the full budget cannot be validated with measured data. Field studies rarely include full N balances, especially N_2 fluxes, which are difficult to quantify. Limiting publication of modeling results based on available field data represents a missed opportunity to improve the understanding of modeled processes. We propose that the modeler community support publication of all simulated N pools and processes in future studies.

Plain Language Summary Biogeochemical models calculate the entire N balance to describe soil N turnover. However, when findings are published, they often focus solely on environmentally harmful N losses like N_2O fluxes and NO_3^- leaching. We argue that it is crucial to publish and communicate the complete N cycle as calculated by the models. This practice is vital for advancing model development, ensuring quality control, facilitating model intercomparison, and generating new hypotheses for empirical field studies. We therefore encourage ecosystem modelers to report all results, even those that cannot be fully validated due to a lack of measurements. We particularly emphasize the importance of denitrification and reporting modeled N_2 fluxes.

1. The Denitrification Data Deficit

1.1. Importance of Denitrification (N_2O and N_2)

To meet the ever-increasing global demand for agricultural products, soil is often augmented using nitrogen (N) fertilizers (Erisman et al., 2011). This significantly impacts the N cycle of agricultural ecosystems and can cause N losses (Davidson, 2012; Galloway et al., 2008; Schlesinger, 2009; Six et al., 2002; Sutton & Bleeker, 2013). Gaseous N losses such as ammonia (NH_3), nitric oxide (NO), nitrous oxide (N_2O), and dinitrogen (N_2), as well as mineral N losses through nitrate (NO_3^-) leaching, impair crop yields and N use efficiency, while contributing to air pollution, global warming, drinking water contamination, eutrophication and acidification of unmanaged

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lands and waters (Galloway et al., 2008). Gaseous soil N losses are associated with the microbial processes of nitrification and denitrification. Nitrification is an aerobic process that oxidizes NH_3 to nitrite (NO_2^-) and NO_3^-, while denitrification is an anaerobic process that reduces NO_3^- to NO_2^-, NO, N_2O, and finally, N_2 (Groffman et al., 2009; Nömmik, 1956). Both processes can be a source of N_2O, a strong greenhouse gas, and reactant in the destruction of stratospheric ozone (Butterbach-Bahl et al., 2013; Canadell et al., 2021; Ravishankara et al., 2009), but denitrification is generally the more substantial N_2O-producing process.

Though our understanding of denitrification in terrestrial ecosystems has improved in recent decades (Galloway et al., 2004; Rohe et al., 2021; Singh et al., 2011; Surey et al., 2021; Zaehle, 2013), it is still far from complete. Agriculture is the main source of anthropogenic N_2O, but we don't completely understand the complex interaction of factors that control how much N is denitrified in arable soils, especially concerning N_2 production. This is a notable knowledge gap. Although N_2O is a greenhouse gas, and N lost as N_2O reduces N availability and the N-use efficiency of crops, the complete reduction to N_2 is a sink for N_2O that decreases the potential for NO_3^- leaching and returns N to the atmosphere, thereby closing the N cycle (Davidson & Seitzinger, 2006). Globally, denitrification rates are associated with large uncertainties, estimated to be 109–573 Tg yr^{-1} (Groffman et al., 2006; Scheer et al., 2020; Schlesinger, 2009), and the lack of data on total denitrification is one of the reasons that N balances can seldom be closed (Allison, 1955). Therefore, we must reduce that uncertainty through a better understanding of denitrification.

The N_2O fluxes of agricultural soils have been the target of intensive worldwide measurement campaigns over the last 20–30 years (Bouwman et al., 2002; Reay et al., 2012; Stehfest & Bouwman, 2006). These studies show that N_2O emissions are event-driven, with high variability both spatially and temporally, responding nonlinearly to environmental parameters, for example, temperature, oxygen (O_2), organic carbon (SOC), pH, freeze/thaw, and NO_3^- availability (Davidson & Swank, 1986; Firestone et al., 1979; Groffman et al., 2009; Rohe et al., 2021; Rummel et al., 2021; Surey et al., 2021; Thomas et al., 1994; Wagner-Riddle et al., 2017; Weier et al., 1993). That level of complexity is challenging to model. Laboratory studies under controlled conditions help isolate specific controlling factors' effects (Grosz et al., 2021; Müller & Clough, 2014; Weier et al., 1993), with both field and laboratory measurements being used to refine biogeochemical models under differing conditions (Deng et al., 2016; Hergoualc'h et al., 2021). However, in many cases, N_2O is neither the final product nor the main product of denitrification (Scheer et al., 2020). The end product is N_2; yet there is no simple field-appropriate method for measuring N_2 (Friedl et al., 2020). The small production from denitrification relative to the high atmospheric background makes measuring soil N_2 fluxes difficult. Therefore, very few in situ measurements of N_2 fluxes are available (Buchen et al., 2016; Ding et al., 2022; Liu et al., 2022; Scheer et al., 2020; Sgouridis et al., 2016; Zistl-Schlingmann et al., 2019).

1.2. Considering N_2 Fluxes in Models

Almost all agronomic and ecological studies of N cycling include model calculations at some scale, with varying complexity. Models are ideally tested and calibrated using measured data, so measured N_2 fluxes are important for model users and developers, yet such data remains limited. Nevertheless, biogeochemical models developed for describing the N cycle of agricultural soils do predict both N_2O and N_2 emissions (Del Grosso et al., 2000; Li et al., 1992; Nylinder et al., 2011; Parton et al., 1996; Sihi et al., 2020). Some models (Del Grosso et al., 2000; Parton et al., 1996) have been partly parameterized with N_2 data that are no longer considered reliable (e.g., based on the acetylene inhibition technique (Weier et al., 1993)) and other model calibrations are simply incomplete. Given the lack of empirical data, approaches to describe soil N_2 are mostly process-oriented, with the sensitivity of both N_2 and N_2O to controlling factors constrained based solely on N_2O data (Grosz et al., 2021; Zhang et al., 2022). In these models, having data from frequent measurements (beyond the common weekly or fortnightly intervals) is crucial. In Saha et al. (2021), a statistical machine learning model was trained on a 3-year, high-frequency N_2O data set and they were able to predict daily N_2O emissions well. However, in many cases, models are not able to consistently and satisfactorily predict daily N_2O emissions. Some models can simulate the cumulative annual emissions, but these approaches often fail to capture the timing and magnitude of observed emission peaks (Frolking et al., 1998).

The inaccuracy of predicted daily N_2O fluxes by biogeochemical models is a well-known problem (Butterbach-Bahl et al., 2013; Zimmermann et al., 2018), partly due to the incomplete understanding of the N_2/N_2O product ratio of denitrification. Since the calibration data and approaches of different models vary, they may produce contrasting

Table 1
The Measured (Laboratory Experiment With ^{15}N Labeling) and Modeled (DNDC, Coup, and DeNi) Average, Cumulative N_2, and N_2O Fluxes (g N ha^{-1}), for an Arable Sandy Soil From Fuhrberg, Germany (Grosz et al., 2021)

	Measured	DNDC	Coup	DeNi
N_2 (g N ha^{-1})	52.63	0.019	155.8	4,607
N_2O (g N ha^{-1})	638.5	345.4	70.15	2,460

Note. The presented results in Table 1 did not cover the statements and results of the entire study by Grosz et al. (2021).

results regarding N_2 emissions, while still predicting similar N_2O emissions. Grosz et al. (2021) compared measured N_2 and N_2O emissions from a laboratory experiment with the results from three models: DNDC, Coup, and DeNi. Note that the models were not calibrated, and that DNDC—without the possibility to manipulate the source code—is not ideal for modeling laboratory experiments. Nevertheless, the modeled N_2O fluxes were not implausible from any of the three models (Table 1). In contrast, the modeled N_2 fluxes by DNDC were almost 3,000 times smaller than the measured data, while those from DeNi were overestimated by a factor of more than 100. While model calibration would have improved the results, this example shows that the additional N_2 flux information is critical for understanding model outputs and identifying potential issues in model estimates of denitrification.

Unfortunately, although many models estimate N_2 fluxes, there are only a few publications presenting modeled N_2 flux results (Del Grosso et al., 2000; Grosz et al., 2021; Leip et al., 2008; Parton et al., 1996). We argue that the publication of total denitrification rates (both N_2 and N_2O), even if N_2 fluxes are not validated, would significantly improve our understanding of different model approaches and aid model development. Models are often used under soil, climate or management conditions that are not fully covered by data sets used for model training and evaluation. Especially in these cases, publishing modeled N_2 fluxes would help to assess the quality and improve the comparability of process descriptions. Presenting only one metabolic intermediate of denitrification, namely N_2O flux, while neglecting N_2 flux, compromises data reliability. Moreover, in the future, as more measured N_2 and N_2O fluxes from field experiments become available, already published simulations of N_2 fluxes will facilitate the uptake and incorporation of new insights.

2. Additional Uncertainties in N Cycle Modeling

2.1. Unknown N-Balances

The inaccuracy of predicted daily N_2O fluxes by biogeochemical models (Butterbach-Bahl et al., 2013; Zimmermann et al., 2018) is not only due to uncertainties in N_2 fluxes, but also due to a lack of knowledge regarding other processes within the N cycle. N_2O fluxes are an integral part of the N cycle, but only represent 0.1%–3.1% of N losses during ecosystem N cycling (Bolan et al., 2004; Bouwman, 1996; Cameron et al., 2013; Clough et al., 2005; Firestone, 1982; Mosier et al., 1998; Thomson et al., 2012). Therefore, they are highly sensitive to other components of the N cycle, including N pools (NH_4^+, NO_3^- or organic N), plant and microbial N immobilization, decomposition, and related N losses like NH_3, NO_x, and NO_3^- leaching. Without going into extensive detail, we emphasize the importance of publishing the full modeled N balance in modeling studies.

Publishing modeled N sources for N_2O fluxes provides information on what pathways the model is simulating (e.g., nitrification or denitrification). Under certain environmental conditions, a model may provide accurate N_2O fluxes even though the underlying processes are incorrect (i.e., be right for the wrong reason); a high degree of equifinality has been shown in previous studies (He et al., 2016). Nitrification is particularly important in this context because in addition to being a source of N_2O, it provides substrate (NO_2^- and NO_3^-) for denitrification. David et al. (2009) simulated an intensively cropped watershed in Illinois using measured water drainage and NO_3^- concentration and compared denitrification from six different models. Most of the models accurately simulated the measured NO_3^- leaching, but the denitrification rates varied widely among the models. This high variation in NO_3^- lost through denitrification would then impact each model's availability of soil NO_3^- for plant and microbial uptake, leaching, and later denitrification. These key differences between models do not become visible without publishing the complete N balance. Finally, having a complete picture of N pools and processes within a model exercise makes it possible to recognize knowledge gaps. In Giltrap et al. (2014), the APSIM and NZ-DNDC models were used for estimating water drainage, NO_3^- leaching, and plant N-uptake from a lysimeter experiment (Giltrap et al., 2014). An important conclusion of their work was that NO_3^- adsorption, a process that was not captured by the models, could influence the whole N cycle and the calculated N balance.

Unlike N_2, there are methods available for the measurement of the other N pools and processes mentioned here. However, given the cost and time that would be necessary to include such a wide array of supporting measurements, few studies (Delon et al., 2017; Janz et al., 2022 are exceptions) can realistically measure all

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N fluxes in parallel, instead focusing on specific N pools and processes of interest. This makes it difficult to compare different studies and to use them for model calibration and evaluation. In a mass balance system, any changes in at one point within the system can significantly affect the entire calculation. This means that we cannot effectively model one or two selected elements of the N cycle separately, but require the whole N balance. And most models calculate the full N balance. We argue here, as we argued above for N_2 fluxes, that publishing unvalidated model output may provide valuable insights into model processes and support the development of models or sub-processes for N cycling.

2.2. Additional Soil Information and Sources of Uncertainty

Ecosystem N cycling does not exist in isolation. Other factors, such as the soil oxygen availability and distribution (Zhang et al., 2022) and labile organic carbon (Philippot et al., 2007), also affect denitrification modeling. Whether a model relates transport functions to water-filled pore space or soil gas diffusivity in order to understand and model soil aeration, can have a significant effect on the simulated N_2O and N_2 production (Balaine et al., 2013, 2016). Similarly, soil gas diffusivity may be used by the model to predict when N_2O and N_2 become entrapped in the soil, rather than released (Clough et al., 2000, 2001; Ding et al., 2022). Available C can strongly influence losses of N and N_2O emissions (Philippot et al., 2007), but accounting for the effects of labile C on N cycling is still a knowledge gap and needs to be better addressed in denitrification modeling (Grosz et al., 2021). Therefore, reporting both model carbon dioxide (CO_2) simulations as well as soil aeration, in addition to N cycling, would considerably improve our understanding of model outputs. Beyond that, we argue that modeling studies with a focus on the C cycle—as with N cycling studies—should report all of the modeled C stocks in soil and vegetation, even without validation (e.g., changes in microbial biomass C and N, rapid dynamics of DOC and DON), for transparency and for future studies. Moreover, in view of the coupling of elemental cycles (Gruber & Galloway, 2008) it is recommended to report not only results of one but rather of all modeled elements, since this would allow cross-checking of elemental mass balances and, for example, verify whether modeled changes in carbon stocks agree with associated mineralization-immobilization of N.

3. Recommendations

We argue that reporting the entire N balance, including unvalidated results like N_2 and other related parameters, should become standard when publishing the results of N model studies. Based on what we outlined above, this would: (a) illustrate the diversity and uncertainty of different modeling approaches, (b) show the robustness of modeled N balances, (c) identify data gaps, and (d) enhance future model development. We assume that the scarcity of "complete" modeled N balances in the soil denitrification literature stems from the reluctance of the scientific community to support the publication of unvalidated modeled output, especially given that the simulation results of these "neglected" N pools may be unrealistic. But this self-censorship of authors has resulted in a missed opportunity to share knowledge and improve our understanding of modeled processes. We recommend that future studies exercise transparency in publishing model outputs. We encourage authors to focus on the aspects of their model that were of particular interest (i.e., validated model developments), but, while clearly stating which variables were not validated by measurements, to include all related pools and parameters to the fullest extent possible. Presenting such results does put additional pressure on the authors, as the presented model outputs have to be sufficiently robust and coherent for publication. However, the publication of the modeled N-balance simulations is crucial for future model development; it would fundamentally improve the robustness of models, speed up fine-tuning, and ultimately advance our understanding of the N cycle.

Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

Data Availability Statement

No data was used in this manuscript.

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