

## Modeling denitrification: can we report what we don't know?

**B. Grosz<sup>1</sup>, A. Matson<sup>2</sup>, K. Butterbach-Bah<sup>3,4</sup>, T. Clough<sup>5</sup>, E. A. Davidson<sup>6</sup>, R. Dechow<sup>1</sup>, S. DelGrosso<sup>7</sup>, E. Diamantopoulos<sup>8</sup>, P. Dörsch<sup>9</sup>, E. Haas<sup>3</sup>, H. He<sup>10</sup>, C. V. Henri<sup>11</sup>, D. Hui<sup>12</sup>, K. Kleineidam<sup>13,14</sup>, D. Kraus<sup>3</sup>, M. Kuhnert<sup>15</sup>, J. Léonard<sup>16</sup>, C. Müller<sup>13,14,17</sup>, S. O. Petersen<sup>18</sup>, D. Sihi<sup>19</sup>, I. Vogeler<sup>18,20</sup>, R. Well<sup>1</sup>, J. Yeluripati<sup>21</sup>, J. Zhang<sup>18</sup>, C. Scheer<sup>3</sup>**

<sup>1</sup>Thünen Institute of Climate-Smart Agriculture, Braunschweig, Germany,

<sup>2</sup>Wageningen University & Research, Wageningen, Netherlands,

<sup>3</sup>Institute of Meteorology and Climate Research Atmospheric Environmental Research (IMK-IFU), Karlsruhe Institute of Technology (KIT), Garmisch-Partenkirchen, Germany,

<sup>4</sup>Department of Agroecology - Center for Landscape Research in Sustainable Agricultural Futures - Land-CRAFT, Aarhus University, Aarhus, Denmark,

<sup>5</sup>Department of Soil & Physical Sciences, Lincoln University, Lincoln 7647, Canterbury, New Zealand,

<sup>6</sup>University of Maryland Center for Environmental Science, MD, USA,

<sup>7</sup>Soil Management and Sugar beet Research Unit, USDA-ARS, CO, USA,

<sup>8</sup>Faculty for Biology, Chemistry, and Earth Science, University of Bayreuth, Bayreuth, Germany,

<sup>9</sup>Faculty of Environmental Sciences and Natural Resource Management, Norwegian University of Life Sciences, Ås, Norway,

<sup>10</sup>Department of Geography, McGill University, Quebec, Canada,

<sup>11</sup>Department of Hydrology, Geological Survey of Denmark and Greenland (GEUS), Copenhagen, Denmark,

<sup>12</sup>Department of Biological Sciences, Tennessee State University, Nashville, TN 37209, USA,

<sup>13</sup>Liebig Centre for Agroecology and Climate Impact Research, Justus Liebig University, Germany

<sup>14</sup>Institute of Plant Ecology, Justus Liebig University Giessen, Germany

<sup>15</sup>Institute of Biological and Environmental Sciences, University of Aberdeen, Aberdeen, AB24 3UU, UK,

<sup>16</sup>BioEcoAgro Joint Research Unit, INRAE, Université de Liège, Université de Lille, Université de Picardie Jules Verne, 02000, Barenton-Bugny, France,

<sup>17</sup>School of Biology and Environmental Science, University College Dublin, Ireland,

<sup>18</sup>Department of Agroecology, Aarhus University, Tjele, Denmark,

<sup>19</sup>Department of Environmental Sciences, Emory University, GA, USA,

<sup>20</sup>Grass Forage Science/Organic Agriculture, Christian Albrechts University, 24118 Kiel, Germany,

<sup>21</sup>Information and Computational Sciences Department, The James Hutton Institute,  
Craigiebuckler, Aberdeen, UK

Corresponding author: Balázs Grosz ([balazs.grosz@thuenen.de](mailto:balazs.grosz@thuenen.de))

**Key Points:**

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

## 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, only specific N pools/fluxes (i.e.  $\text{N}_2\text{O}$ ,  $\text{NO}_3^-$ ,  $\text{NH}_3$ ,  $\text{NO}_x$ ) are usually published, because the full budget cannot be validated with measured data. Field studies rarely include full N balances, especially  $\text{N}_2$  fluxes, which are difficult to quantify. Limiting publication of modeling results based on available field data is a missed opportunity to improve the understanding of modeled processes. We suggest 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, but published results are generally limited to environmentally harmful N losses like  $\text{N}_2\text{O}$  fluxes and  $\text{NO}_3^-$  leaching. We argue that the publication and presentation of the full N cycle calculated by the model are crucial for model development, quality control, model intercomparison, and generating new hypothesis for empirical field studies. We therefore encourage ecosystem modelers to report all relevant results, even those that cannot be fully validated due to a lack of measurements. We particularly emphasize the importance of denitrification and reporting modeled  $\text{N}_2$  fluxes.

## 1 The denitrification data deficit

### 1.1 Importance of denitrification ( $\text{N}_2\text{O}$ and $\text{N}_2$ )

Denitrification is an anaerobic metabolic process for energy production in soils driven by the soil microbial community. It describes the step-wise reduction of nitrate ( $\text{NO}_3^-$ ) to nitrite ( $\text{NO}_2^-$ ), nitric oxide (NO), nitrous oxide ( $\text{N}_2\text{O}$ ), and finally, dinitrogen ( $\text{N}_2$ ) as the end product (Groffman et al., 2009; Nömmik, 1956). Although our knowledge and understanding of denitrification in terrestrial ecosystems has increased in recent decades (Galloway et al., 2004; Singh et al., 2011; Zaehle, 2013), we still have limited knowledge of the complex interaction of the many controlling factors, especially with respect to  $\text{N}_2$  production.

Denitrification is a key N transformation process in soil, with both positive and negative consequences. On the one hand, it is a source of  $\text{N}_2\text{O}$ , a strong greenhouse gas, and reactant in the destruction of stratospheric ozone (Canadell et al., 2021; Ravishankara et al., 2009; Robertson, 2000) and reduces ecosystem N availability and N use efficiency of agricultural crops. On the other hand, complete reduction to  $\text{N}_2$  is a sink for  $\text{N}_2\text{O}$ , and N loss via this pathway decreases the possibility of  $\text{NO}_3^-$  leaching, returning N to the atmosphere and closing the N cycle (Davidson & Seitzinger, 2006). Globally, denitrification rates are associated with large uncertainties, estimated to be in the range of 109-573 Tg yr<sup>-1</sup> (Groffman et al., 2006; Scheer et al., 2020; Schlesinger, 2009). The lack of data on total denitrification has long been recognized as one of the reasons that N balances can seldom be closed at the plot scale (Allison, 1955). Given the importance of this for the N balance of terrestrial ecosystems, it is vital that we reduce uncertainty through a better understanding of the denitrification process.

The  $\text{N}_2\text{O}$  fluxes of agricultural soils are well documented and regularly measured, with 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  $\text{N}_2\text{O}$  emissions are event

driven, with high variability both spatially and temporally, responding nonlinearly to environmental parameters, e.g., 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; Mørkved et al., 2006; Nömmik, 1956; Thomas et al., 1994; Wagner-Riddle et al., 2017; Weier et al., 1993). This level of complexity is challenging to model. Laboratory studies under controlled conditions help to isolate the effects of specific controlling factors (Grosz et al., 2021; Müller & Clough, 2014; Weier et al., 1993), with both field and laboratory measurements being used to refine biogeochemical models to calculate  $N_2O$  flux under differing conditions (Deng et al., 2016; Hergoualc'h et al., 2021). Much effort has been made to monitor, understand, and model  $N_2O$  emissions, but  $N_2O$  is neither the final product, nor in many cases the main product, of denitrification (Scheer et al., 2020). The end product of denitrification is  $N_2$ . Unlike  $N_2O$  fluxes, measuring  $N_2$  fluxes from the soil is fraught with difficulties due to the relatively small production from denitrification compared to the high atmospheric background. While several methods exist for measuring  $N_2$  fluxes, each has its own shortcomings, and there is no simple field-appropriate method (Friedl et al., 2020). 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

Models are tested and calibrated using measured data, so access to measured  $N_2$  fluxes is important for model developers. But those data are simply not yet available in sufficient quantity. Biogeochemical models have nevertheless been developed for describing the N cycle of agricultural soils and predicting  $N_2O$  and  $N_2$  emissions (Del Grosso et al., 2000; Li et al., 1992; Nylander 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 data that are no longer considered reliable (e.g.,  $N_2$  loss estimation on basis of the acetylene inhibition technique (Weier et al., 1993)) and other model calibrations are simply incomplete.

Given the lack of data to generate empirical models, approaches to describe the production and transport of  $N_2$  are mostly process-oriented. Denitrification models are highly diverse with regard to their complexity, but the sensitivity of both  $N_2$  and  $N_2O$  to controlling factors (e.g. temperature,  $pO_2$ , SOC, pH, freeze/thaw and  $NO_3^-$  availability) is commonly constrained solely based on  $N_2O$  data (Grosz et al., 2021; Zhang et al., 2022). Yet it is notable that even given the extensive  $N_2O$  data available, no statistical or process-based model has been found that can 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), and 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 results regarding  $N_2$  emissions, while still creating similar  $N_2O$  emissions. Grosz et al. (2021) compared measured  $N_2$  and  $N_2O$  emissions from a laboratory experiment with modeled results from the process-based models DNDC and DeNi. It is important to note that the models were not calibrated and DNDC – without the possibility to manipulate the source code –

is not ideal for modeling laboratory experiments. Nevertheless, as shown in Table 1, the modeled  $\text{N}_2\text{O}$  fluxes from both models were acceptable, with DNDC producing results of the same magnitude as measured fluxes, while DeNi produced fluxes four times higher, but not implausible. In contrast, the modeled  $\text{N}_2$  fluxes by DNDC were almost 3000 times smaller than the measured data, while those from DeNi were overestimated by a factor of more than 100. While model calibration would clearly have improved those results, this example shows that the additional  $\text{N}_2$  flux information is critical for understanding model outputs and identifying implausible model estimates of denitrification.

**Table 1.** The measured (laboratory experiment with  $^{15}\text{N}$  labeling) and modeled (DNDC and DeNi) average, cumulative  $\text{N}_2$ ,  $\text{N}_2\text{O}$  fluxes ( $\text{g N ha}^{-1}$ ), for arable sandy soil from Fuhrberg, Germany (Grosz et al., 2021).

	Measured	DNDC	DeNi
$\text{N}_2$ [ $\text{g N ha}^{-1}$ ]	56.63	0.019	7067
$\text{N}_2\text{O}$ [ $\text{g N ha}^{-1}$ ]	638.5	345.4	2460

Unfortunately, although many models estimate  $\text{N}_2$  fluxes, there are only a few publications presenting modeled  $\text{N}_2$  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  $\text{N}_2$  and  $\text{N}_2\text{O}$ , reported on the same time scale), even if  $\text{N}_2$  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  $\text{N}_2$  fluxes would help to assess the quality and improve the comparability of process descriptions. Presenting only one metabolic intermediate of denitrification, namely  $\text{N}_2\text{O}$  flux, while neglecting  $\text{N}_2$  flux, compromises data reliability. Moreover, in the future, as more measured  $\text{N}_2$  and  $\text{N}_2\text{O}$  fluxes from field experiments become available, already published simulations of  $\text{N}_2$  fluxes will facilitate the uptake and incorporation of new insights.

## 2 Additional uncertainties in denitrification modeling

### 2.1 Unknown N-balances

The inaccuracy of predicted daily  $\text{N}_2\text{O}$  fluxes by biogeochemical models (Butterbach-Bahl et al., 2013; Zimmermann et al., 2018) is not only due to uncertainties in  $\text{N}_2$  fluxes, but also due to a lack of comprehensive understanding of other processes within the N cycle.  $\text{N}_2\text{O}$  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; Bouwman et al., 1993; Bremner, 1997; Cameron et al., 2013; Clough et al., 2005; de Klein et al., 2001; Firestone, 1982; Freney, 1997; Haynes & Sherlock, 1986; Mosier et al., 1998; Saggar et al., 2009; Thomson et al., 2012). Therefore, they are highly sensitive to other components of the N cycle, including N pools ( $\text{NH}_4^+$ ,  $\text{NO}_3^-$  or organic N), plant and microbial N immobilization, decomposition, and related N losses like  $\text{NH}_3$ ,

NO<sub>x</sub>, and NO<sub>3</sub><sup>-</sup> leaching. Without going into extensive detail, we emphasize here the importance of publishing the full modeled N balance in denitrification studies.

Publishing modeled N sources for N<sub>2</sub>O 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<sub>2</sub>O 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<sub>2</sub>O, it provides substrate (NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup>) for denitrification. David et al. (2009) simulated an intensively cropped watershed in Illinois using measured water drainage and NO<sub>3</sub><sup>-</sup> concentration and compared denitrification from six different models (David et al., 2009). Most of the models accurately simulated the measured NO<sub>3</sub><sup>-</sup> leaching, but the denitrification rates varied widely among the models. This high variation in NO<sub>3</sub><sup>-</sup> lost through denitrification would then impact each model's availability of soil NO<sub>3</sub><sup>-</sup> for plant and microbial uptake, leaching, and later denitrification. These key difference 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<sub>3</sub><sup>-</sup> leaching, and plant N-uptake from a lysimeter experiment (Giltrap et al., 2014). An important conclusion of their work was that NO<sub>3</sub><sup>-</sup> adsorption, a process that was not captured by the models, could influence the whole N-cycle and the calculated N balance.

Unlike N<sub>2</sub>, there are available methods 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 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 validation. We argue here, as we argued above for N<sub>2</sub> 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 the success of modeling N<sub>2</sub>O and N<sub>2</sub> production. For example, 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<sub>2</sub>O and N<sub>2</sub> production (Balaine et al., 2013, 2016). Similarly, soil gas diffusivity may be used by the model to predict when N<sub>2</sub>O and N<sub>2</sub> become entrapped in the soil, rather than released (Clough et al., 2000, 2001; Ding et al., 2022). Studies show that available C can strongly influence losses of N and N<sub>2</sub>O emissions (Philippot et al., 2007), but accounting for labile C 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<sub>2</sub>) simulations as well as soil aeration in addition to N cycling simulation results would considerably improve understanding of model outputs.

## 3 Recommendations

Although our main focus here is on the importance of reporting both N<sub>2</sub> and N<sub>2</sub>O fluxes when modeling denitrification, we argue that including the entire N balance and related

parameters should become standard when publishing the results of N model studies. Based on what we outlined above, this would: 1) enhance future model development, 2) allow to assess the robustness of modelled N balances, 3) illustrate the diversity and uncertainty of the different approaches for modeling denitrification processes in soils, and 4) identify data gaps that should be addressed in future studies.

We assume that the scarcity of “complete” (i.e. including N<sub>2</sub> fluxes and other N pools/pathways) 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 ask 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 (e.g. all modeled N pools/pathways, soil aeration and CO<sub>2</sub> flux). 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.

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