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Estimating fractions of N_2O emissions from nitrification and denitrification using data assimilation

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Abstract: Nitrous oxide (N_2O) is a potent greenhouse gas contributing to global warming and stratospheric ozone depletion. N_2O is primarily produced through nitrification and denitrification, which are regulated by soil and environmental factors. Numerous studies have been conducted to investigate nitrification and denitrification processes, their controlling factors and their contributions to N_2O production. However, it is still challenging to estimate the parameters of process-based models based solely on limited experimental data. For example, although modules of N_2O emissions from different pathways have been included in most process-based models, some parameters such as the ratio of N_2O derived from nitrification and denitrification have not been well estimated. A fixed ratio is used in these models to estimate the proportion of N_2O emissions from nitrification and denitrification. Moreover, the relationships between nitrification, denitrification, their associated N_2O emissions and potential key drivers remain unclear and have been handled inconsistently in existing process-based models. These unknowns may also result in uncertain predictions of feedback to different N management practices and environmental conditions.

The application of nitrification inhibitors (NIs) e.g., 3-methylpyrazole 1,2,4-triazole (3MPTZ), 3,4-dimethylpyrazole phosphate (DMPP), acetylene (C_2H_2) is widely used to reduce N_2O emissions. NIs could delay the oxidation of NH_4^+ to hydroxylamine, the first step of nitrification, thus decreasing the amount of NO_3^-, which is susceptible to leaching and loss through denitrification. While many process-based models simulate N_2O emissions, their capacity to represent NIs' impact on N cycling is constrained by the lack of an NI module and relevant parameters.

Data assimilation enhances the model accuracy and reliability by optimizing model representation to align with observational data. Through the integration of mathematical process models and empirical experimental data, data assimilation is expected to enhance ecological forecasting by estimating parameters and their uncertainties that are not directly measurable through experiments. However, the application of data assimilation has not been extended to the N_2O emission simulation. This technique can enhance performance of N_2O modelling by optimizing difficult-to-measure parameters and reducing model uncertainty.

In this study, we incorporated data assimilation into a coupled carbon–nitrogen model to estimate soil nitrification, denitrification, N_2O emissions, and their related parameters under various soil moisture levels (Water-filled pore space (WFPS) at 50% and 70%), incubation temperature (15, 25 and 35°C) and nitrification inhibitor application (DMPP, 3MPTZ and C_2H_2) in cereal and vegetable production systems in Australia.

We found that the contribution of nitrification to N_2O emissions (i.e., the fraction of N_2O emitted from nitrification, f_{N2O_nit}) decreased with increasing temperature and moisture content, whereas denitrification dominated N2O production (i.e., the fraction of N_2O emitted from denitrification, f_{N2O_dni}) under 70% WFPS regardless of temperatures. Under fertilizer N application, the use of nitrification inhibitors decreased f_{N2O_nit}) but increased f_{N2O_dni}). The efficacy of nitrification inhibitors in mitigating N_2O emissions varied with environmental conditions. In this study, we demonstrate the use of data assimilation to constrain key parameters for predicting nitrification, denitrification and associated N_2O emissions in response to soil environments and management practices. Integrating this technique into ecosystem process-based models has the potential to enhance model accuracy by reducing uncertainties and biases.

Keywords: *Data assimilation, N_2O production, nitrification, denitrification, model parameter*