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Parameterizing an agricultural production model for simulating nitrous oxide emissions in a wheat-maize system in the North China Plain

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ABSTRACT

Concentrations of atmospheric nitrous oxide (N_2O), a potent greenhouse gas, have been continuously increasing, and cropland soils are one of the largest sources of N_2O . Variations in environmental and anthropogenic factors have substantial impacts on both the frequency and magnitude of N_2O emissions. Based on measurements from a wheat-maize system in the North China Plain, the authors parameterized the Agricultural Production Systems Simulator (APSIM) model, which was initially developed in Australia, for simulating N_2O emissions under different agricultural management practices. After calibrating one of the key parameters — the fraction of N_2O lost in nitrification (k_2) — the results showed that the model successfully captured the daily N_2O fluxes under different nitrogen fertilization treatments, but underestimated some large peak fluxes. By pooling all data together, the calibrated APSIM model also performed well in representing cumulative N_2O emissions under various treatments at annual and finer (monthly and daily) time scales.

摘要

农田土壤是大气氧化亚氮的一个重要排放源,农田氧化亚氮的排放同时受到气候环境和人为 活动的复杂影响。本文基于中国华北平原的一个农田试验站的观测数据,对农业生产模拟器 (APSIM)进行参数化,并检验该模型在不同时间尺度上模拟农田氧化亚氮排放的能力。结果 表明,对消化系数(k,)进行校正后,模型能够较好地模拟不同时间尺度和不同施肥处理下小 麦-玉米系统的土壤氧化亚氮排放,但是对于一些较高的峰值排放模拟效果欠佳。

1. Introduction

Nitrous oxide (N₂O) is a potent greenhouse gas that, on the basis of mass, absorbs much more infrared radiation than carbon dioxide and methane. The atmospheric concentrations of N₂O increased significantly in the last century (from ~275 ppbv in 1900 to ~317 ppbv in 2000), mainly as a result of anthropogenic factors (Mosier and Kroeze 2000). As a highly managed system, cropland soil is one of the largest emitters of N₂O at the global scale. In 2010, agriculture was estimated to contribute 70% of global N₂O emissions (Olivier, Janssens-Maenhout, and Peters 2012). Cropland soil N₂O emissions are determined mainly by microbial processes of nitrification and denitrification, which are further regulated by agricultural practices, as well as edaphic and climatic conditions (Li 2000; Mosier and Kroeze 2000). For example, Huang et al. (2002) reported that soil texture influences soil organic matter decomposition rates, thereby potentially regulating the

amount of substrates used by microbes to produce N₂O. Zheng et al. (2000) reported that soil moisture is also a sensitive factor involved in the regulation of N₂O emissions from agricultural soils. Climatic factors such as temperature and precipitation also play an important role in agricultural N₂O production (Meng, Cai, and Ding 2005). Additionally, agricultural practices such as nitrogen amendments from fertilizer and manure, cultivation, tillage regime, irrigation, and cropping systems, also tend to alter N₂O emission rates (Del Grosso et al. 2009). The complex interactions between agricultural practices and environmental conditions hinder our ability to accurately predict changes in N₂O emissions over time and space. The modelling approach enables exploration of the interactions between climate, soil conditions, and management practices as they regulate soil biophysical and biochemical processes. Many process-based models, such as DNDC (Denitrification-Decomposition; Li 2000), DAYCENT (daily version of the CENTURY model;

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Parton et al. 1994), and Agricultural Production Systems Simulator (APSIM; Keating et al. 2003), have been developed and widely used to quantify the effects of environmental and anthropogenic changes on N₂O emissions (Thorburn et al. 2010; Cheng et al. 2014; Cui et al. 2014). For simulation outputs to be credible, together with accurate climatic and edaphic observations, detailed information on agricultural management (such as the cropping system, fertilizer application, irrigation, and tillage intensity) is required. In addition, validating the model's performance against field experimental observations is also an essential prerequisite.

APSIM was developed in Australia for modelling plant and soil processes and has been widely used to study crop productivity, nutrient cycling, and the environmental effects of farming systems as influenced by climate change and management interventions (van Ittersum, Howden, and Asseng 2003; Luo et al. 2011, 2013). In our previous work, we parameterized the model for simulating crop productivity and soil organic carbon dynamics in the typical upland soils in northern regions of China (Wang et al. 2014, 2015). However, the model's performance in simulating N₂O emissions has yet to be tested in China's croplands, where nitrogen fertilizers have been intensively applied and the associated N₂O emissions are of wide concern (Ju et al. 2009). The aim of the present study was to parameterize APSIM for simulating N₂O emissions in a typical wheat-maize system in the North China Plain.

2. Field experiment site description

A wheat-maize rotation field experimental site (Figure 1) located in the eastern areas of the North China Plain was



Figure 1. Location of the study site.

selected for this study. The information on climate, soil, agricultural management practices, and annual cumulative N₂O emissions were obtained from Cui et al. (2012) and Yan et al. (2013, 2015). The N₂O fluxes at finer temporal resolutions (e.g. daily or every 2-3 days) were measured in situ using the closed chamber method The study region has a warm temperate continental monsoon climate, and the mean annual temperature and average annual precipitation are 13.0 °C and 586 mm, respectively (Yan et al. 2015). The soil has a silt-loam texture in the cultivated layer, the initial bulk density was 1.42 g cm⁻³, and the soil organic carbon and total nitrogen content were 10.28 and 1.05 g kg⁻¹, respectively (Yan et al. 2015). Before the experiment, the region had been cultivated with a double cropping system of winter wheat and summer maize rotation for more than 50 years.

The field experiment lasted two years following its commencement in October 2008. In total, three nitrogen fertilizer level treatments were arranged as follows: (a) a control treatment without nitrogen application (CK); (b) the farmer's conventional nitrogen dose (CP) of 600 kg N ha^{-1} yr⁻¹ (with 45% for wheat and 55% for maize); and (c) the optimal practice with a reduced nitrogen dose (UA), which was 1/3 lower than CP, and recommended by local agronomists (Yan et al. 2015). Under each treatment, three replicate plots (51 m² for each) were randomly chosen within a uniform area that had been cultivated with a wheat-maize rotation system under conventional practices before the experiments (Yan et al. 2013). For the CP and UA treatments, nitrogen fertilization was adopted twice for each crop growing season: around half the amount of nitrogen fertilizer was applied before or immediately after sowing, and the other half during wheat tillering or when maize plants had 11-12 leaves (Cui et al. 2012). In the experiments, topsoil moisture was measured daily with a portable moisture probe (ML2x, ThetaKit, Delta-T Devices, Cambridge, UK). The amount of irrigation water used in each event was manually determined. Under each treatment, static chambers as well as gas chromatography techniques (Wang and Wang 2003) were used to collect air samples for measuring the N₂O fluxes (Yan et al. 2013). The normal sampling frequency was once a week during winter and once every three to four days during other seasons. Intensified daily sampling was carried out following events that were likely to stimulate intensive N₂O emissions, such as fertilizer application, irrigation, rainfall, and tillage (Cui et al. 2012). The annual total N₂O emissions were calculated by integrating the observed and gap-filled daily fluxes, i.e. daily fluxes of the observational intervals were estimated as the arithmetic means of neighboring data (Yan et al. 2013). More detailed information on the field experiment can be found in Cui et al. (2012) and Yan et al. (2013, 2015).

3. APSIM model description

APSIM is a biophysical and biochemical model used to study productivity and nutrient cycling of agroecosystems as influenced by environmental and anthropogenic variations (Keating et al. 2003). APSIM simulates crop growth and soil carbon and nitrogen processes on a daily timescale in response to climate (i.e. temperature, rainfall, and radiation), soil water availability, and soil nutrient status. In the model, direct N₂O emissions from the soil are simulated as the sum of N₂O emissions from the processes of denitrification and nitrification. Denitrification (R_{denit} ; units: kg N ha⁻¹ d⁻¹) is estimated as a function of the amount of nitrate (NO₃; units: kg N ha⁻¹), the concentration of active carbon (C_{A} ; units: ppm), soil temperature (T), and moisture (M):

$$R_{\text{denit}} = k_{\text{denit}} \times \text{NO}_3 \times C_A \times T \times M$$

where k_{denit} is the denitrification coefficient, with a default value of 0.0006. N₂O emissions from denitrification are then estimated as a fraction of total denitrified nitrogen using the ratio of nitrogen gas (N₂) to N₂O emitted during denitrification. The N₂/N₂O_{denit} ratio is mainly related to gas diffusivity in soil at field capacity (k_1), the nitrate concentration of the soil on a dry weight basis, and the heterotrophic CO₂ respiration rate (Thorburn et al. 2010). Nitrification is determined by Michaelis–Menten kinetics, which is further modified by soil pH, soil moisture, and temperature. A fraction of the nitrified nitrogen is emitted as N₂O (k_2 , with a default value of 0.002). A detailed model description can be found in Keating et al. (2003), and the routines involved in N₂O emissions from soil are described in Thorburn et al. (2010).

4. Model parameterization

Daily weather data, including maximum and minimum temperatures, precipitation, and radiation, are required as model inputs. The climate data were obtained from the nearest meteorological station (Weifang Station) to the experimental site (http://www.cdc.cma.gov.cn/). The daily radiation was estimated from the daily sunshine duration using the Angström formula (Jones 1992). Soil hydraulic parameters (Figure 2) such as saturated water content, drained upper limit, 15-bar lower limit, and lower limit of crop water extraction, were calculated based on the method of Luo et al. (2011). Using the method of Wang et al. (2015), the total soil carbon content at the start of the experiments was used to initialize the soil carbon pools in APSIM. The flows between various pools were calculated in terms of carbon, and the nitrogen flows were determined based on the carbon to nitrogen ratio of the corresponding pool. The parameters involved in wheat and maize growth



Figure 2. Soil hydraulic parameters at the study site. SAT, saturation water content; DUL, drained upper limit; LL15, 15-bar lower limit; LL, lower limit of crop water extraction. LL is equal to LL15, resulting in the merger of the two lines.

were adopted from Wang et al. (2015) because of the similar study region, cropping system, and soil and climate conditions. Following Shi et al. (2013), an equilibrium run forcing the same one-year (2008–09) data was not stopped until the soil carbon pools reached a steady state for the model initialization.

For the processes involved in denitrification and nitrification, following Thorburn et al. (2010), we set k_{denit} and k_1 as the default values, while calibrating k_2 to obtain the best matches between the model outputs and the observations. This is because, in APSIM, denitrification parameters have been optimized against observed data, whereas k_2 is acknowledged to be soil-specific (Thorburn et al. 2010). Based on the minimum RMSE method of Cheng et al. (2014), we calculated the RMSE to assess the main difference between the observations and simulations, as follows:

$$\mathsf{RMSE} = \sqrt{\sum_{i=1}^{n} \frac{(P_i - O_i)^2}{n}}$$

where *P* and *O* represent the model estimates and field measurements, respectively; \overline{O} is the mean of observed N₂O emissions (kg N ha⁻¹ yr⁻¹), and *n* is the total number of observations. By setting an increment of 0.0001 for k_2 , the model was run for all values of k_2 within the range 0–0.005. We ultimately obtained a k_2 value of 0.0023 that resulted in a best match between the observed and predicted N₂O emissions. This was acceptable because the fraction of N₂O



Figure 3. The (a) daily precipitation and amount of irrigation, (b) nitrogen fertilization rates, and (c) observed vs. simulated soil moisture, under the farmer's conventional practice at the Huantai experimental site.

lost in nitrification can be adjusted and it normally varies from 0.001 to 0.05 (Goodroad and Keeney 1984).

5. Results and discussion

5.1. Model simulation for the wheat-maize system in the North China Plain

We begin by presenting the important environmental controls on N_2O fluxes (Figure 3). Figure 3(a) shows the daily precipitation and amount of water irrigation for the study site. Only the nitrogen fertilization rates under the CP treatment were available, which are also presented in Figure 3(b). Since the soil moisture is a direct factor influencing N_2O fluxes, we also compared the seasonal variations of observed and simulated soil moisture (Figure 3(c)). The model generally captured the seasonal variations of soil moisture well, but there were still some discrepancies between daily simulated and observed values (Figure 3(c)).

Additionally, the observed and predicted daily N_2O fluxes from October 2008 to October 2010 were compared (Figure 4). The results of the two fertilized treatments, i.e. the farmer's conventional nitrogen dose (CP) of 600 kg N ha⁻¹ yr⁻¹ and the optimal practice with a reduced nitrogen dose (UA) that was 1/3 lower than the CP, are presented. The observed daily N_2O fluxes were highly variable within each rotation under the two treatments (Figure 4).



Figure 4. Observed and simulated daily fluxes of N_2O from (a) the farmer's conventional nitrogen dose (CP) of 600 kg N ha⁻¹ yr⁻¹, and (b) the optimal practice with a reduced nitrogen dose (UA), which was 1/3 lower than the CP treatment, at the Huantai site during 2008–2010.

Note: The black and blue lines show observations and predictions, respectively.

Observed peaks in N₂O emissions (Figure 4(a)) usually took place following fertilization, irrigation (especially after fertilizer application), and heavy rainfall (Figures 3(a) and (b)). For example, during late-June 2009 and mid-August 2010, heavy rainfall accompanied the fertilization-induced N₂O peaks (Figures 3(a), (b), and 4). This is consistent with the findings of previous studies, in which it was indicated that nitrogen fertilization and irrigation or heavy rainfall events jointly stimulate much more intensive N₂O emissions (Yan et al. 2015). The potential mechanism is that nitrogen fertilization provides a substrate for the processes involved with nitrification and denitrification; plus, irrigation and precipitation regulate soil moisture (Figure 3(c)), which further affects the activity of nitrifiers and denitrifiers in producing N₂O. The highest fluxes under both the CP and UA treatments were observed during the second maize season, which were induced by heavy rainfall events immediately following urea top-dressing. Compared with observations, APSIM generally captured the temporal pattern of daily N₂O fluxes quite well, although it underestimated the peak N₂O fluxes caused by irrigation following fertilization in October 2008 for both treatments (Figure 4). Overall, the results shown in Figure 4 indicate that the model was able to simulate the N₂O fluxes over time.

By configuring APSIM with detailed observations of soil, climate, and agricultural management, the model performed well in reproducing the annual cumulative N₂O emissions under the CK, CP, and UA treatments when all data were pooled together (Figure 5(a)). The model simulation resulted in an R² (a widely used goodness-of-fit measure that ranges from 0 to 1 where 1 represents a perfect fit) and RMSE value of 0.74 and 0.95 kg ha⁻¹, respectively, in terms of annual N₂O emissions. These results indicate that the model performs well in representing the annual cumulative N₂O emissions under different treatments of nitrogen fertilization. Figure 5(b) shows the modeled vs. observed N₂O emissions at the monthly scale during the study period. In general, the calibrated APSIM model was also able to reasonably represent the monthly cumulative N₂O emissions under different nitrogen fertilization treatments ($R^2 = 0.79$; RMSE = 0.28 kg ha⁻¹). On the daily timescale (Figure 5(c)), negative biases existed between the modeled and observed N₂O fluxes, especially for the peak fluxes. The regression between the simulated and observed daily N_2O fluxes resulted in an R^2 value of 0.34, with a slope of 0.45 and an intercept of 0.01 kg ha^{-1} . The RMSE between the daily simulated and observed values was 0.04 kg ha⁻¹.



Figure 5. Comparison of observed and simulated (a) annual, (b) monthly and (c) daily cumulative N_2O emissions under different treatments from the wheat–maize rotation cropping system at Huantai site during the study period of 2008–2010.

In general, although there were some discrepancies between the daily modeled and observed fluxes, the model was generally able to simulate the annual N_2O emissions under different conditions. Thus, it may also be applicable to larger regions with similar cropping systems, soil and climate conditions across the agroecosystems in the North China Plain.

5.2. Limitations and future needs

In simulating agricultural soil N₂O emissions, the APSIM model does possess some shortcomings that should be noted when interpreting our results. First, the model underestimated some peak N₂O fluxes compared with observations (Figure 4). In fact, this is a common problem in this field (Smith et al. 2008; Chirinda et al. 2011; Lehuger et al. 2011; Bell et al. 2012; Cui et al. 2014; Zhang et al. 2015). For example, DNDC, Landscape DNDC and IAP-N-GAS also cannot capture N₂O peaks for croplands in China (Figure 6 in Cui et al. 2014; Zhang et al. 2015; Figure 3). A similar pattern in the comparison between simulated and observed daily N₂O fluxes was also shown in Bell et al. (2012), who used the ECOSSE model to simulate N₂O emissions from a maize-wheat-barley crop rotation system (compare Figure 5(c) in this study and Figure 5(a) in Bell et al. (2012)). In Lehuger et al. (2011), the CERES-EGC model significantly underestimated the N₂O peaks at a European cropland site. The reasons for the low capability of present models in capturing N₂O dynamics have been discussed in previous studies (Zhang et al. 2015). Firstly, both the guantity and activity of soil microbes involved in the processes of nitrification and denitrification may differ under different environmental conditions, and yet this aspect is not included in most process-based models, including APSIM. Secondly, models reflect the knowledge gap with respect to the complex interactions among the soil moisture

content, organic matter decomposition, and soil nitrogen availability (Zhang et al. 2015). This is a challenging line of enquiry for model modifications and development in the future. Incorporating a module involving soil microbe quantities and activity, and advancing model capacity to better represent the complex interactions among soil moisture, organic matter decomposition and soil nitrogen availability, may help to fill this gap. As a result, the effects of events connected with soil N₂O production still need to be explicitly addressed in future research, in order to better simulate N₂O fluxes under different conditions of environmental and anthropogenic change.

Secondly, the model also yielded some small peak fluxes that were not observed (Figure 4). This may have been due to the inadequate air sampling frequency and intense observations only having been carried out following events that were likely to stimulate intensive N₂O emissions (Cui et al. 2012). Therefore, intensified air sampling on a daily basis throughout the study period is a necessary step in future field experiments.

Although discrepancies existed in the magnitudes of some peak N_2O emissions (Figure 4), the process-based model successfully captured the temporal pattern of daily N_2O emissions (Figure 4) and accumulative N_2O emissions at both annual and monthly scales (Figure 5). This indicates the importance of process-based modeling approaches, because quantifications of N_2O emissions and mitigation potential on relatively large spatial and temporal scales are a key concern in both scientific and political spheres.

6. Conclusion

N₂O emissions are highly dependent on environmental changes (e.g. heavy rainfall) and anthropogenic factors such as fertilizer application, irrigation, and tillage. The parameterized APSIM model captured the daily N₂O fluxes

well under different nitrogen fertilization treatments in a wheat-maize system in the North China Plain, but underestimated some peak fluxes. By pooling all data together, the model performed well in reproducing the cumulative N₂O emissions under various treatments at annual, monthly, and daily scales.

Disclosure statement

No potential conflict of interest was reported by the authors.

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