RESEARCH ARTICLE

Enhancing the soil and water assessment tool model for simulating N_2O emissions of three agricultural systems

Qichun Yang,[1] Xuesong Zhang,[1,2,7] Michael Abraha,[2,3] Stephen Del Grosso,[4] G. P. Robertson,[2,3,5] and Jiquan Chen[2,6]

[1]Joint Global Change Research Institute, Pacific Northwest National Laboratory, College Park, Maryland 20740 USA
[2]Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, Michigan 48824 USA
[3]W.K. Kellogg Biological Station, Michigan State University, Hickory Corners, Michigan 49060 USA
[4]Agricultural Research Service, United States Department of Agriculture, Fort Collins, Colorado 80526 USA
[5]Department of Plant, Soil, and Microbial Sciences, Michigan State University, East Lansing, Michigan 48824 USA
[6]Department of Geography, Environment, and Spatial Sciences, Michigan State University, East Lansing, Michigan 48824 USA

Abstract. Nitrous oxide (N_2O) is a potent greenhouse gas (GHG) contributing to global warming, with the agriculture sector as the major source of anthropogenic N_2O emissions due to excessive fertilizer use. There is an urgent need to enhance regional-/watershed-scale models, such as Soil and Water Assessment Tool (SWAT), to credibly simulate N_2O emissions to improve assessment of environmental impacts of cropping practices. Here, we integrated the DayCent model's N_2O emission algorithms with the existing widely tested crop growth, hydrology, and nitrogen cycling algorithms in SWAT and evaluated this new tool for simulating N_2O emissions in three agricultural systems (i.e., a continuous corn site, a switchgrass site, and a smooth brome grass site which was used as a reference site) located at the Great Lakes Bioenergy Research Center (GLBRC) scale-up fields in southwestern Michigan. These three systems represent different levels of management intensity, with corn, switchgrass, and smooth brome grass (reference site) receiving high, medium, and zero fertilizer application, respectively. Results indicate that the enhanced SWAT model with default parameterization reproduced well the relative magnitudes of N_2O emissions across the three sites, indicating the usefulness of the new tool (SWAT-N_2O) to estimate long-term N_2O emissions of diverse cropping systems. Notably, parameter calibration can significantly improve model simulations of seasonality of N_2O fluxes, and explained up to 22.5%–49.7% of the variability in field observations. Further sensitivity analysis indicates that climate change (e.g., changes in precipitation and temperature) influences N_2O emissions, highlighting the importance of optimizing crop management under a changing climate in order to achieve agricultural sustainability goals.

Key words: *agriculture; climate change; greenhouse gas; sensitivity analysis.*

Citation: Yang, Q., X. Zhang, M. Abraha, S. Del Grosso, G. P. Robertson, and J. Chen. 2017. Enhancing the soil and water assessment tool model for simulating N_2O emissions of three agricultural systems. Ecosystem Health and Sustainability 3(2):e01259. doi: 10.1002/ehs2.1259

Introduction

Increasing greenhouse gas emissions have raised growing concerns about their potential warming impacts on the global climate system (Lashof and Ahuja 1990, Solomon et al. 2009). Although the concentration of N_2O in the atmosphere is much lower than that of CO_2 and CH_4 (Flückiger et al. 1999), N_2O plays a disproportionately important role in contributing to global warming due to a long atmospheric lifetime (Ko et al. 1991) that contributes to its high global warming potential (Lashof and Ahuja 1990). In addition, N_2O is the primary ozone-depleting gas in the stratosphere (Ravishankara et al. 2009). The agriculture sector is the major source of anthropogenic N_2O emissions due to excessive fertilizer use (Reay et al. 2012).

N_2O emissions are regulated by numerous factors including soil nitrogen contents, soil temperature, soil water, and quality of organic residues (Firestone et al. 1980, Novoa and Tejeda 2006, Butterbach-Bahl et al. 2013). Production of N_2O through reduction of nitrate (NO_3^-) and oxidation of ammonia (NH_4^+) is directly controlled by levels of the two inorganic nitrogen species. Excessive nitrogen input via chemical fertilizer application has been considered as a key driver for the high N_2O emissions from agricultural ecosystems (Thomson et al. 2012). However, non-linear correlations between fertilizer application and N_2O emissions suggested that additional factors, such as soil temperature and moisture, may add variability

Manuscript received 13 November 2016; revised 30 December 2016; accepted 3 January 2017.
[7]**E-mail:** xuesong.zhang@pnnl.gov

to the response of N_2O production to fertilizer addition (Kim et al. 2013*b*). Microbial activities during nitrification and denitrification tend to be more active under higher temperatures (Kätterer et al. 1998), suggesting that air temperature plays an important role in the seasonal patterns of N_2O fluxes (Rezaei Rashti et al. 2015). Soil water content is another factor with significant role in regulating N_2O emissions. Water-filled pore space (WFPS) determines the reduction and oxidation environment in soils and thus controls the relative contribution of nitrification and denitrification to total N_2O emissions (Bateman and Baggs 2005). Other factors, such as soil pH, soil carbon (Shcherbak et al. 2014), and soil texture, also impact N_2O emissions, either through regulating microbial activities or through affecting soil water content (Weier et al. 1993).

Investigating the confounding impacts of multiple environmental factors on N_2O emissions is critical for enriching understanding of N_2O production, emission, and mitigation (Deng et al. 2016, Liu et al. 2016). Numerical modeling investigations are important in complementing and extrapolating field observations. While model simulation experiments are useful in disentangling the complex interactions among different environmental factors and ecological processes (Yang et al. 2015, Yang and Zhang 2016), process-based algorithms have been developed and applied to quantify contributions of multiple processes and factors to N_2O emissions, as well as to project N_2O emissions under alternative climate and management scenarios (Del Grosso et al. 2008, Abdalla et al. 2010, Rafique et al. 2014). There is an urgent need to enhance regional-/watershed-scale agricultural models to simulate N_2O emissions to complement their existing strengths in assessing impacts of cropping practices on soil quality, soil erosion, and water quality.

The Soil and Water Assessment Tool (SWAT, Arnold et al. 1998) has been widely applied to assess impacts of crop cultivation on biogeochemical cycling (El-Khoury et al. 2015), hydrological dynamics (Wu et al. 2012, Leta et al. 2015), and environmental pollutions (Holvoet et al. 2008). Recent efforts (Zhang et al. 2013) incorporated the CENTURY model (Parton et al. 1994) into SWAT to simulate residue-soil organic matter (SOM) dynamics. N_2O production and subsequent emissions are, however, not represented in the model, limiting application of SWAT to provide comprehensive assessment of agricultural activities on nitrogen cycling.

Our primary objective of this study was to improve SWAT's representation of soil nitrogen cycling by modifying its nitrification and denitrification algorithms and adding N_2O emission algorithms. Specifically, we integrated the DayCent model's nitrification, denitrification, and N_2O production modules (Del Grosso et al. 2000) with the existing widely tested crop growth, hydrology, and nitrogen cycling processes in the SWAT. We tested this new tool for simulating N_2O emissions at three cropping sites (i.e., a continuous corn site, a switchgrass site, and a reference site dominated by smooth brome grass) located in the Great Lakes Bioenergy Research Center (GLBRC) scale-up fields in southwestern Michigan. A local parameter sensitivity analysis was conducted to understand how N_2O estimates respond to changes in key parameters. We also analyzed how changes in precipitation and temperature affect N_2O emissions. This work strengthens SWAT's capability to provide comprehensive assessment of sustainability of agricultural ecosystems under a changing climate.

Methods

Integrating DayCent's N_2O emission algorithms into SWAT

The SWAT N_2O emission algorithms are based on Parton et al. (2001) that simulate N_2O production from both nitrification and denitrification. Specifically, soil ammonia oxidation is simulated with the following equations:

$$N_{\text{nit}} = f_{\text{moist}} \times f_{\text{st}} \times f_{\text{pH}} \times N_{\text{nit\_max}} + N_{\text{nit\_base}} \quad (1)$$

$$f_{\text{moist}} = \frac{1}{1 + 30 \times e^{-9 \times \text{rel\_wc}}} \quad (2)$$

$$rel_{\text{wc}} = \frac{\frac{\text{SW}}{\text{STH}} - \text{SW}_{\text{mim}}}{\frac{\text{FC}}{\text{STH}} - \text{SW}_{\text{mim}}} \quad (3)$$

$$\text{SW}_{\text{mim}} = \frac{\text{WP}}{\text{STH}} - \text{SW}_{\text{del}} \quad (4)$$

$$f_{\text{st}} = e^{\frac{4.5 \times (1 - (\frac{-5 - \text{ST}}{-40})^7) \times (\frac{-5 - \text{ST}}{-40})^{4.5}}{7}} \quad (5)$$

$$f_{\text{pH}} = 0.56 + \frac{1}{\pi} \times \text{atan}\,(\pi \times 0.45 \times (\text{SPH} - 5)) \quad (6)$$

$$N_{\text{nit\_max}} = f_{\text{nit\_max}} \times \text{NH4}, \quad (7)$$

where N_{nit} is soil nitrification rate (g $N \cdot m^{-2} \cdot d^{-1}$); f_{moist} represents impacts of soil water on nitrification, and f_{st} represents soil temperature impacts; f_{pH} refers to the pH impacts on nitrification; SW is soil water content (mm H_2O); STH is soil depth (mm); WP is soil moisture at wilting point (mm H_2O); FC is soil moisture at field capacity (mm H_2O); SW_{mim} is minimum volumetric soil water content (unitless); SW_{del} is minimum volumetric soil water content below wilting point (0.042, unitless); ST is soil temperature (Celsius degree); SPH refers to soil pH; NH4 is soil ammonia content (g N/m^2); $N_{\text{nit\_max}}$ is maximum nitrification rate (0.4 g $N \cdot m^{-2} \cdot d^{-1}$); N_{nit} is denitrification rate (g $N \cdot m^{-2} \cdot d^{-1}$); $N_{\text{nit\_base}}$ is minimum nitrification rate (0.00001 g $N \cdot m^{-2} \cdot d^{-1}$); $f_{\text{nit\_max}}$ is maximum fraction of ammonia that is nitrified during nitrification (unitless).

N_2O production from nitrification is calculated as a fraction of nitrified ammonia:

$$E_{\text{N2O\_nit}} = f_{\text{N2O\_to\_nit}} \times N_{\text{nit}} \quad (8)$$

$$f_{\mathrm{N2O\_to\_nit}} = \frac{adj_{\mathrm{wp}} - adj_{\mathrm{fc}}}{dDO_{\mathrm{wp}} - dDO_{\mathrm{fc}}} \times \left(dDO_{\mathrm{sf}} - dDO_{\mathrm{wp}}\right) + adj_{\mathrm{wp}}, \quad (9)$$

where $E_{\mathrm{N2O\_nit}}$ is N_2O production from nitrification (g $N{\cdot}m^{-2}{\cdot}d^{-1}$); $f_{\mathrm{N2O\_to\_nit}}$ is the ratio of N_2O to nitrified ammonia (unitless); adj_{fc} is maximum ratio of N_2O production to nitrified N at field capacity (calibrated parameter, unitless); adj_{wp} is minimum ratio of N_2O production to nitrified ammonia at wilting point (calibrated parameter, unitless); dDO_{fc} and dDO_{wp} are normalized diffusivity in soil at field capacity and wilting point, respectively (unitless); dDO_{sf} refers to the normalized diffusivity of the top soil layer (unitless). More details about calculation of the diffusivity factors are provided in the supporting information.

Following Parton et al. (2001) and Del Grosso et al. (2000), we also revised SWAT to simulate N_2O production from denitrification, which is influenced by soil nitrate content, temperature, soil water, and soil respiration:

$$E_{\mathrm{N2O\_den}} = \frac{E_{\mathrm{den}}}{1 + Rn2n2o} \quad (10)$$

$$Rn2n2o = \mathrm{fRno3\_co2} \times \mathrm{fRwfps} \quad (11)$$

$$\mathrm{fRno3\_co2} = \left(38.4 - 350 \times dD0_{\mathrm{fc}}\right) \times e^{\frac{-0.8 \times nppm}{co2ppm}} \quad (12)$$

$$fRwfps = 1.5 \times wfps - 0.32 \quad (13)$$

$$E_{\mathrm{Nden}} = Dtotflux \times fDwfps \times C_{\mathrm{unit}} \times \rho_{\mathrm{soil}} \quad (14)$$

$$Dtotflux = \min\left(fDco2, fDno3\right) \quad (15)$$

$$fDco2 = 0.1 \times \mathrm{co2}_{\mathrm{correction}}{}^{1.3} - min\_nit \quad (16)$$

$$fDno3 = 1.556 + \frac{79.92}{3.14} \times \mathrm{Arctan}\left(3.14 \times 0.0022 \times \left(nppm - 9.23\right)\right) \quad (17)$$

$$fDwfps = \frac{0.45 + \left(\mathrm{atan}\left(0.6 \times \mathrm{PI} \times 10 \times \left(wfps - x\_inflextion\right)\right)\right)}{\pi} \quad (18)$$

$$wfps = \frac{\mathrm{swcfrac}}{\mathrm{porosity}} \quad (19)$$

$$x_{\mathrm{inflextion}} = \left(9 - M \times \mathrm{co2}_{\mathrm{correction}}\right) \times wfps\_adj \quad (20)$$

$$M = dD0_{\mathrm{fc}} \times (-1.25) + 0.145 \quad (21)$$

$$\mathrm{co2}_{\mathrm{correction}} = co2ppm \times \left(1 + aa \times \left(wfps - wfps_{\mathrm{threshold}}\right)\right. \quad (22)$$

$$co2ppm = \frac{\mathrm{respc}}{\rho_{\mathrm{soil}}} \quad (23)$$

$$aa = \begin{cases} 0.8 & \text{when } dD0_{\mathrm{fc}} \geq 0.15 \\ -0.1 \times dD0_{\mathrm{fc}} + 0.019 & \text{when } dD0_{\mathrm{fc}} < 0.15 \end{cases}, \quad (24)$$

where $E_{\mathrm{N2O\_den}}$ is N_2O production rate through nitrification on a given day (g $N{\cdot}m^{-2}{\cdot}d^{-1}$); E_{N2O} is denitrification rate (g $N{\cdot}m^{-2}{\cdot}d^{-1}$); $Rn2n2o$ is ratio of N_2 to N_2O (unitless); $fRno3\_co2$ represents CO_2 effect on the ratio of N_2 to N_2O (unitless); $wfps$ is water-filled pore space (unitless); $nppm$ is soil nitrate content (ppm N/m^2); $co2\ ppm$ is CO_2 concentration in soils (ppm); C_{unit} is a conversion coefficient to change unit from ppm to g/g (10^{-6}); ρ_{soil} is soil density (g soil/cm^3); $Dtotflux$ is the denitrified nitrogen (ppm N/d); $fRwfps$ represents effect of $wfps$ on the ratio of N_2 to N_2O (unitless); $fDwfps$ represents effect of $wfps$ on denitrification; $fDco2$ is denitrification rate due to CO_2 concentration (ppm N/d); $fDno3$ is denitrification flux due to soil nitrate (ppm N/d); $x_{\mathrm{inflextion}}$ denotes impacts of CO_2 concentration on $fDwfps$ (unitless); $co2_{\mathrm{correction}}$ is corrected CO_2 concentration (ppm); min_nit is minimum nitrate concentration required in a soil layer for trace gas calculation (ppm N); $respc$ is soil respiration (g $C{\cdot}m^{-2}{\cdot}d^{-1}$); $wfps_{\mathrm{threshold}}$ is a threshold value for water-filled pore space (unitless); $wfps\_adj$ is the adjustment on inflection point for water-filled pore space effect on denitrification curve (unitless); aa denotes impacts of soil diffusivity on soil CO_2 concentrations (unitless); M is an intermediate parameter in calculating $x_{\mathrm{inflextion}}$ (unitless); $dD0_{\mathrm{fc}}$ is normalized soil diffusivity at field capacity (unitless). Details about calculation of this variable are introduced in the supporting information.

Nitric oxide (NO) is a byproduct of the nitrification process and is also produced during the denitrification reaction sequence (Robertson and Groffman 2015). Because the DayCent algorithm does not explicitly represent all of the biochemical steps that occur during nitrification and denitrification, NO is calculated based on modeled N_2O production and a NO/N_2O ratio function. The function is based on the assumption that higher gas diffusivity and increased O_2 availability will lead to higher NO emissions. We used the following equations to simulate NO emission following the DayCent model (Parton et al. 2001):

$$E_{\mathrm{NO\_N2O}} = \left(E_{\mathrm{N2O\_den}} + E_{\mathrm{N2O\_nit}}\right) \times R_{\mathrm{no\_n2o}} \quad (25)$$

$$R_{\mathrm{no\_n2o}} = 8 + \frac{18 \times \mathrm{Arctan}(0.75 \times \pi \times (10 \times dD0)}{\pi}, \quad (26)$$

where $E_{\mathrm{NO\_N2O}}$ is the NO flux converted from N_2O (g $N{\cdot}m^{-2}{\cdot}d^{-1}$); $R_{\mathrm{no\_n2o}}$ is the ratio of NO to N_2O (unitless); $dD0$ is the normalized soil diffusivity (unitless).

Data collection

We collected observational data from three GLBRC sites, namely continuous corn, switchgrass, and smooth brome

grass (reference site) from the Marshall Farm scale-up experimental fields (Fig. 1). These cropping systems were established in 2009 to study how production of different biofuel crops affects biodiversity and biogeochemistry in this region (Zenone et al. 2011). In 2009, the corn and switchgrass sites were planted with soybean and were converted to corn and switchgrass in 2010, respectively. The smooth brome grass site (reference site) is unmanaged and treated as a reference site. Variables selected to evaluate model performance include soil moisture, N_2O fluxes, and crop yields. Soil moisture data were collected twice a year from 2009 to 2013 at the three sites. During each sampling period, ten replicates were collected at each site. Soil samples from the composite of the top 25 cm were collected and sent to laboratory for further analysis. Soil moisture was calculated as the difference between the fresh weight and the dry weight of soil samples (https://data.sustainability.glbrc.org/protocols/24). At the selected sites, N_2O measurements were conducted during 2009–2014. Before 2013, gas samples were collected biweekly during growing seasons (April–November); after 2013, sampling frequency was increased to weekly in June. N_2O was measured using in situ closed-cover flux chambers (https://data.sustainability.glbrc.org/protocols/113). Four replicates were installed at each site to minimize random errors during sampling. Corn and switchgrass were harvested in October or November, and yield data for the two crops during 2010–2014 were collected to evaluate SWAT simulations of crop yields at the corn and switchgrass sites. More details about the data collection and sample analysis can be obtained from GLBRC data catalog (https://data.sustainability.glbrc.org/datatables).

Model setup, calibration, and performance evaluation

Although SWAT is a watershed-scale model, it allows for treating a hydrologic response unit as a land unit representing detailed characteristics of agroecosystems. Latitude/longitude and elevation of the selected sites were downloaded directly from the GLBRC website (http://lter.kbs.msu.edu/datatables/286). Daily climate data (precipitation, temperature, solar radiation, wind, and relative humidity) observed at the Kellogg Biological Station (KBS) were obtained from the KBS LTER database (http://lter.kbs.msu.edu/datatables) from 1993 to 2014. We used the Soil Survey Geographic Database (SSURGO) downloaded from the Geospatial Data Gateway (https://gdg.sc.egov.usda.gov/) to obtain soil properties, including soil layer depth, soil texture, soil bulk density, and soil organic carbon content for each site. Model simulations were conducted from 1993 to 2014, with 1993–2008 as model initialization, while model performance evaluation was mainly focused on the period of 2010–2014, when observed data were available.

We first simulated N_2O fluxes at the three sites with default parameters from the DayCent model. Then, we adjusted key model parameters regulating N_2O production through nitrification and denitrification manually to minimize the discrepancies between model estimates and field observations. The optimized parameters with least bias in N_2O simulations were used to generate calibrated model estimates for the test sites (Table 1).

We evaluated model performance at multiple temporal scales. First, we examined model simulations of soil moisture over the selected sites for those days with field observations. Next, we compared model estimates with observed N_2O fluxes at the monthly scale. Observed N_2O fluxes from 2010 to 2014 were linearly interpolated to obtain daily fluxes, and then, we aggregated the gap-filled data to the monthly scale for model performance evaluation. We also evaluated model-simulated multiple-year average crop yields for the harvested corn and switchgrass sites.

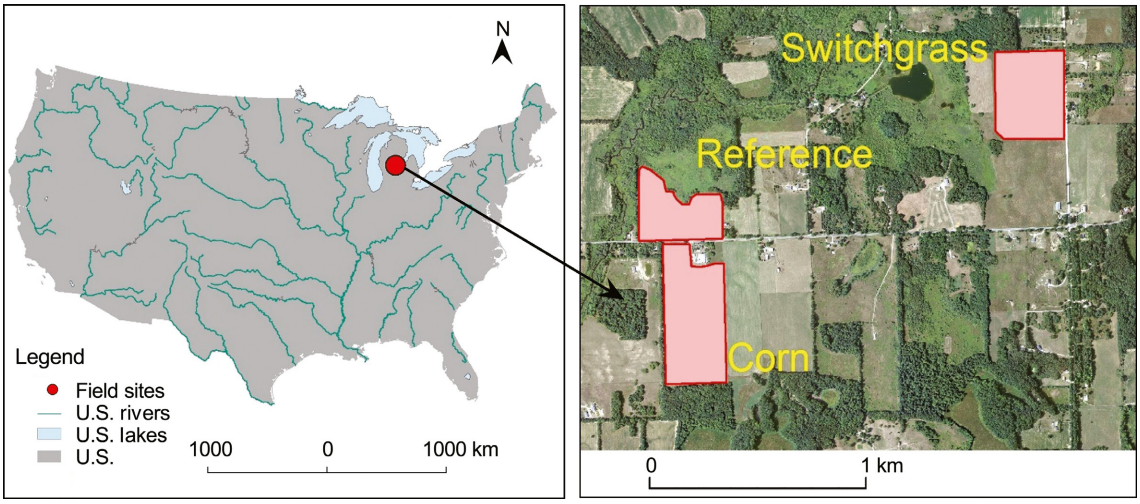

Fig. 1. Location of three GLBRC scale-up experiment sites used for this study. Field observations from 2010 to 2014 were compiled for model performance evaluation.

Table 1. Key SWAT parameters controlling N_2O emissions in nitrification and denitrification.

Parameters	Unit	Default values	Calibrated values	Range from previous studies	References
adj_{fc}	Unitless	0.015	0.012–0.018	0.0–1.0	Bell et al. (2012) Parton et al. (2001)
adj_{wp}	Unitless	0.002	0.0019–0.0022	0.0–1.0	Parton et al. (2001)
wfps_adj	day^{-1}	1	1.1–1.3	0.75–1.3	Del Grosso (Pers. Comm.)
min_nit	Unitless	0.1	0.1	0.05–0.1	Parton et al. (2001)
f_{nit_max}	Unitless	0.15	0.13–0.17	0.0–1.0	Parton et al. (2001)

Notes: adj_{fc} is maximum fraction of N_2O to nitrified N at the field capacity; adj_{wp} is minimum fraction of N_2O to nitrified nitrogen at the wilting point; *wfps_adj* is adjustment on inflection point for water-filled pore space effect on denitrification curve (unitless); *min_nit* is minimum nitrate concentration required in a soil layer for trace gas calculation (ppm N); f_{nit_max} is maximum fraction of ammonia that is nitrified during nitrification (unitless). Range of *wfps_adj* was obtained through personal communication with Dr. Del Grosso.

Sensitivity analysis

We conducted a local parameter sensitivity analysis for five key parameters (Table 1). Here, we assumed that all the selected parameters are normally distributed. We increased and decreased, respectively, the calibrated optimum values of these parameters by 20% to assess the sensitivity of all five parameters. Results of such an analysis were expected to provide valuable information for future calibration and application of the algorithms.

We also evaluated how SWAT N_2O estimates respond to changes in precipitation and temperature to understand how possible climate scenarios would affect N_2O emissions. We increased and decreased daily precipitation by 20% to represent future wet and dry climate scenarios, respectively; we increased daily air temperature by 1° and 2°C to represent future warming scenarios.

Results

Model performance evaluation

Previous investigations demonstrated that soil moisture has significant impacts on N_2O emissions. Reasonable simulation of soil moisture is an important prerequisite for reliably simulating N_2O fluxes. For most days with available field observations, simulated soil moisture was close to the mean or within one standard deviation of observation (Fig. 2), indicating that SWAT-estimated soil moisture matches well observations. Discrepancies between model estimates and observations, particularly for days with intensive rainfall events, should be further reduced through more comprehensive parameter calibration in the future.

With the default parameter values, SWAT simulated well the magnitude of average N_2O emissions of the three cropping systems (Fig. 3). Specifically, the estimated growing-season N_2O emission rate during 2010–2014 at the corn site was 1.08 ± 0.82 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$ (mean ± standard deviation), which was very close to the observed magnitude of 1.10 ± 2.58 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$. At the switchgrass site, model-estimated and observed average N_2O fluxes were 0.22 ± 0.10 and 0.16 ± 0.13 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$, respectively. At the unmanaged reference site that had much lower N_2O emissions than the corn and switchgrass sites, modeled N_2O emissions of 0.08 ± 0.05 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$ also corresponded well to the observed fluxes of 0.05 ± 0.04 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$. Overall, the default parameter settings could generally reflect the differences in the magnitude of N_2O emissions across the three sites. The default parameterization also captured well temporal patterns in N_2O fluxes at the two managed sites (corn and switchgrass sites), for which modeled and observed N_2O fluxes were significantly ($P < 0.1$) correlated. At the reference site, the default simulation failed to reproduce seasonal patterns of N_2O emissions at a significance level of 10% ($P > 0.1$).

Calibration of key parameters substantially improved the model performance (Figs. 4 and 5), in particular for further reducing biases in estimated magnitude of N_2O fluxes at the reference and switchgrass sites. Specifically, parameter adjustment further decreased the bias at the switchgrass site to 15.1%. For the reference site, discrepancies between observations (0.05 ± 0.04 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$) and simulations (0.04 ± 0.02 kg $N{\cdot}ha^{-1}{\cdot}month^{-1}$) were reduced to 23% (Fig. 5), as compared to a 54% bias in the default simulation.

Apart from matching the magnitude, parameter adjustment achieved better representations of the seasonal patterns in N_2O emissions than default simulations. Correlations between simulated and observed monthly N_2O fluxes were improved and significant at the monthly scale across all sites ($P < 0.05$). N_2O emissions were much higher during growing season, particularly from May to August, than during non-growing season. At the corn and switchgrass sites, both modeled and observed N_2O fluxes increased rapidly from April to May and reached peak values in May and June. Then, N_2O emissions decreased substantially from July to November. At the reference site, model simulations corresponded well with observations regarding the decreasing trend of N_2O fluxes from June to November.

Across the three sites with different levels of management intensity, we attained a significant correlation between simulated N_2O fluxes and field observations (Fig. 6). The model simulations explained 22.53% of the variability in N_2O emissions across three sites, confirming the feasibility of employing the new algorithms

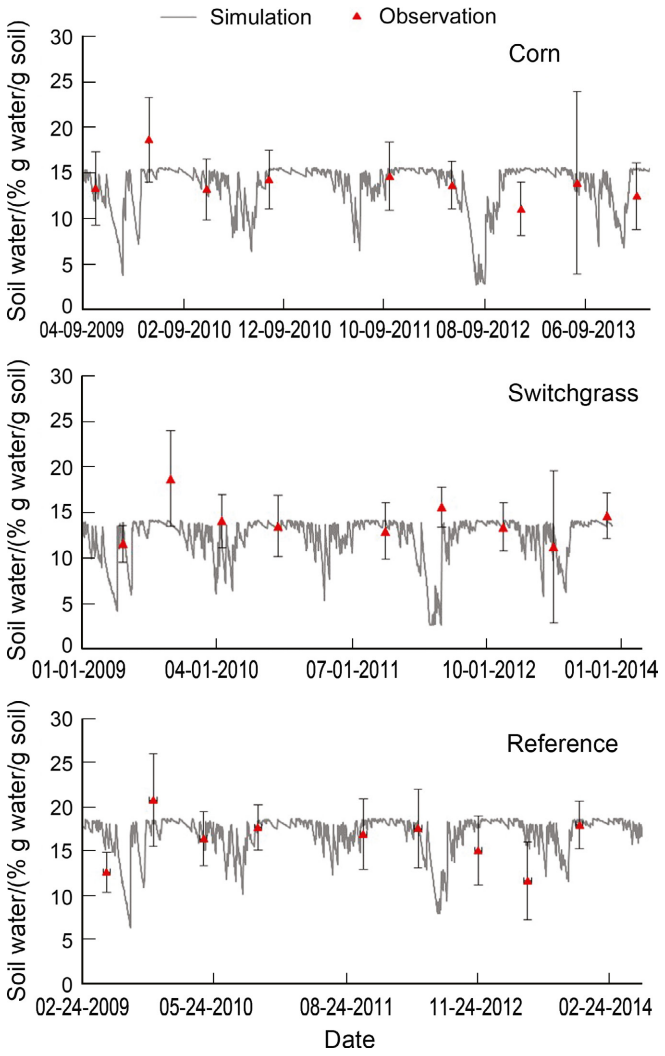

Fig. 2. Comparison of simulated and observed soil water content across the three sites. Soil moisture data were collected twice a year from 2009 to 2013 at the three sites. For days with available data, average soil moisture and its standard deviation were obtained from ten replicates at each site.

to evaluate influences of agricultural activities on N_2O emissions across diverse agricultural ecosystems. Note that when the month with extremely high N_2O emissions was excluded in the model-data comparison, the model would explain 49.7% of the variability in N_2O fluxes (Fig. 6).

SWAT simulated well crop yields at the corn and switchgrass sites. Specifically, at the corn site, our estimate of crop yields during 2010–2014 was 7.96 ± 1.85 Mg/ha, which was comparable to the observations of 7.51 ± 3.25 Mg/ha. Model-estimated switchgrass yields of 7.89 ± 1.36 Mg/ha agreed well with the observations of 7.50 ± 2.56 kg/ha during 2011–2014.

Sensitivity analysis

We selected five parameters that are closely related to N_2O emissions to examine the responses of simulated N_2O fluxes to a 20% change (increase or decrease) of each parameter at the three sites (Table 2). N_2O emissions positively correlated with maximum fraction of N_2O to nitrified N at the field capacity (adj_{fc}) and minimum fraction of N_2O to nitrified nitrogen at the wilting point (adj_{wp}), but had negative correlations with adjustment on inflection point for water-filled pore space effect on denitrification curve (*wfps_adj*). Specifically, with a 20% reduction of adj_{fc}, N_2O emissions were reduced by 9.41%, 12.19%, and 12.68% for corn, switchgrass, and reference sites, respectively; in contrast, a 20% increase in adj_{fc} increased N_2O fluxes by 9.21% at the corn site, 12.14% at the switchgrass site, and 12.69% at the reference site. In response to changes (±20%) in adj_{wp}, simulated N_2O emissions varied from a reduction of 0.19% to an increase of 0.17% at the corn site. Similarly, responses at the switchgrass site to this parameter ranged from 0% to 0.38%. At the reference site, N_2O emissions were reduced by 0.72% with a 20% decrease in adj_{wp}, but increased by 0.72% in response to a 20% increase in this parameter. Adjustments (±20%) of minimum nitrate content (*min_nit*) in soil for denitrification had insignificant influence on N_2O emissions at the two managed sites (changes are less than 0.1%), but induced more sensitive responses (−0.72% to 0.2% changes) at the reference site.

Simulated N_2O emissions were sensitive to changes in *wfps_adj* as well. At the corn site, a 20% increase in *wfps_adj* reduced N_2O emission estimates by 40.48%, whereas a 20% decrease in this parameter increased model-estimated N_2O fluxes by 86.79%. At the switchgrass site, model estimates varied from −33.65% to +18.14% with ±20% changes of this parameter. At the reference site, a 20% increase in *wfps_adj* decreased modeled N_2O emissions by 3.9%, whereas a 20% reduction substantially increased N_2O emissions by 195.1%. Responses of N_2O emissions to the maximum fraction of ammonia that is nitrified during nitrification (f_{nit_max}) varied across the selected sites. At the corn and reference sites, a 20% increase in f_{nit_max} boosted increases in N_2O emissions by 2.35% and 0.53%, respectively, whereas a 20% reduction resulted in decreases of 3.62% and 0.77%, respectively. At the switchgrass site, the response of N_2O emissions was less sensitive to ±20% changes in f_{nit_max}, ranging from −0.19% to 0.18%.

Climatic influences

Changing climate conditions affected N_2O emissions (Table 3). Our sensitivity analysis suggested that N_2O emissions had positive responses to changes in precipitation. With a 20% increase in precipitation, N_2O emissions would increase by 1.39%, 1.50%, and 1.44% at the corn, switchgrass, and reference sites, respectively, whereas under the drier scenario (a 20% reduction in precipitation), N_2O fluxes would be reduced by 3.66%, 3.12%, and 1.52%, respectively. Higher temperatures would generally increase N_2O emissions. With a 1°C increase in air

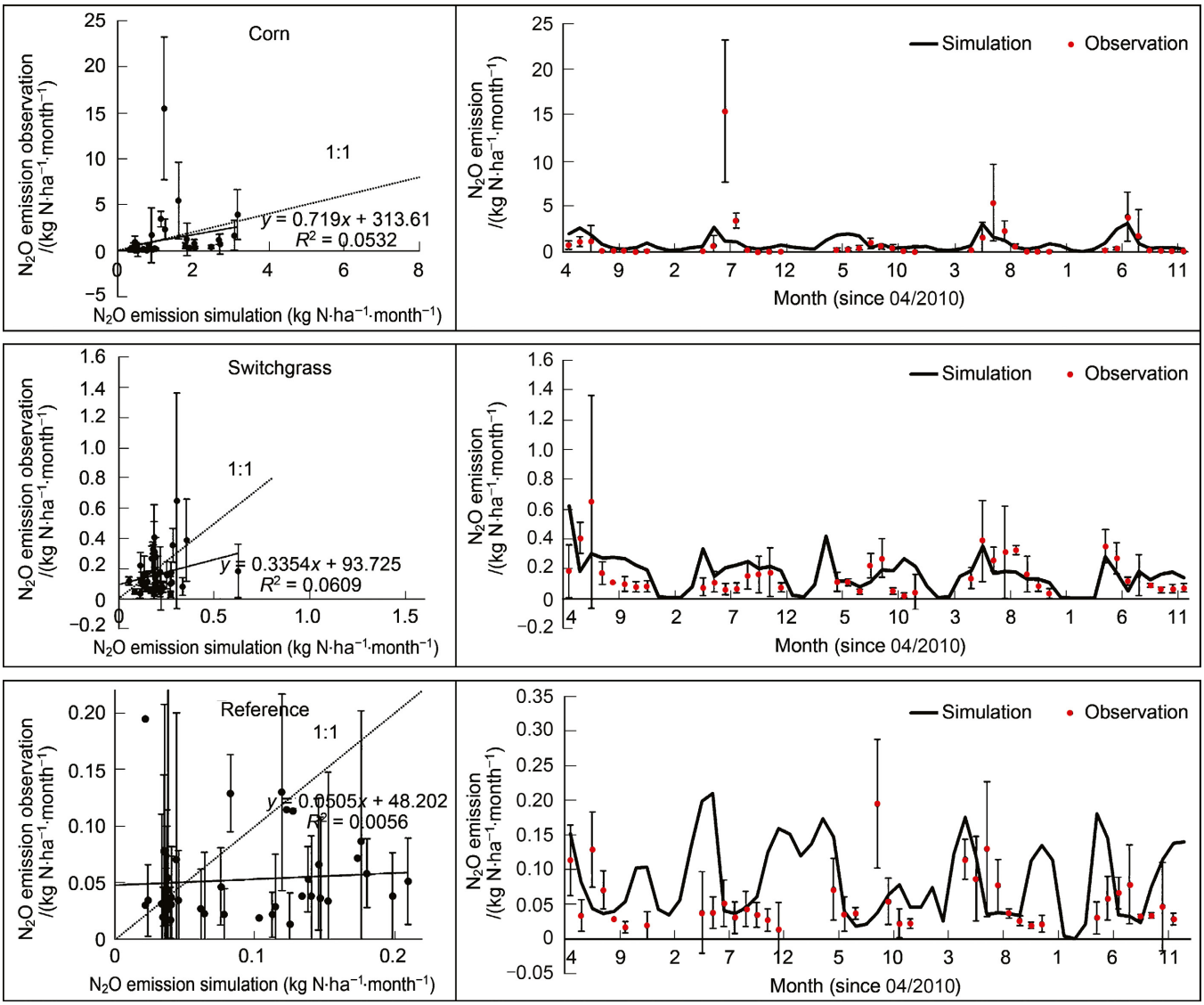

Fig. 3. Model estimates of N_2O emissions compared with default SWAT simulations at the three sites. In this comparison, observed N_2O fluxes were linearly interpolated and aggregated to obtain monthly fluxes.

temperature, N_2O emissions would be enhanced by 1.94–3.69% across the three sites. A 2°C increase would further increase N_2O emissions by 14.4% and 5.74% at the corn and reference sites, respectively, but the switchgrass would only increase by 0.59%.

Discussion

Enhanced SWAT for simulating N2O emissions

As a potent GHG, increasing emissions of N_2O from terrestrial ecosystems to the atmosphere has raised concerns about its potential impacts on the climate system (Butterbach-Bahl et al. 2013). Significant efforts have been devoted to investigating N_2O fluxes from cropland since agricultural land has been identified as a key contributor of the anthropogenic N_2O emissions (Del Grosso et al. 2009). Numerical simulation of N_2O fluxes is critical for predicting N_2O emissions under different management scenarios, and provides valuable information for the mitigation practices (Del Grosso et al. 2009). By integrating the DayCent N_2O emission algorithms with SWAT's existing crop growth, hydrology, and biogeochemical cycling algorithms, we created a new modeling tool that allows us to include N_2O emissions as an important dimension in watershed-scale assessment of sustainability of agricultural ecosystems.

Model evaluation shows that the new module provided reasonable estimates of N_2O fluxes across sites with divergent management intensities, as well as reproduced the seasonal patterns of N_2O emissions. Accuracy of model prediction in this study is close to the previous modeling efforts based on the DayCent model and the DeNitrification–DeComposition (DNDC) model (Parton et al. 2001, Abdalla et al. 2010, Rafique et al. 2013, Grant et al. 2015), indicating feasibility of applying the new

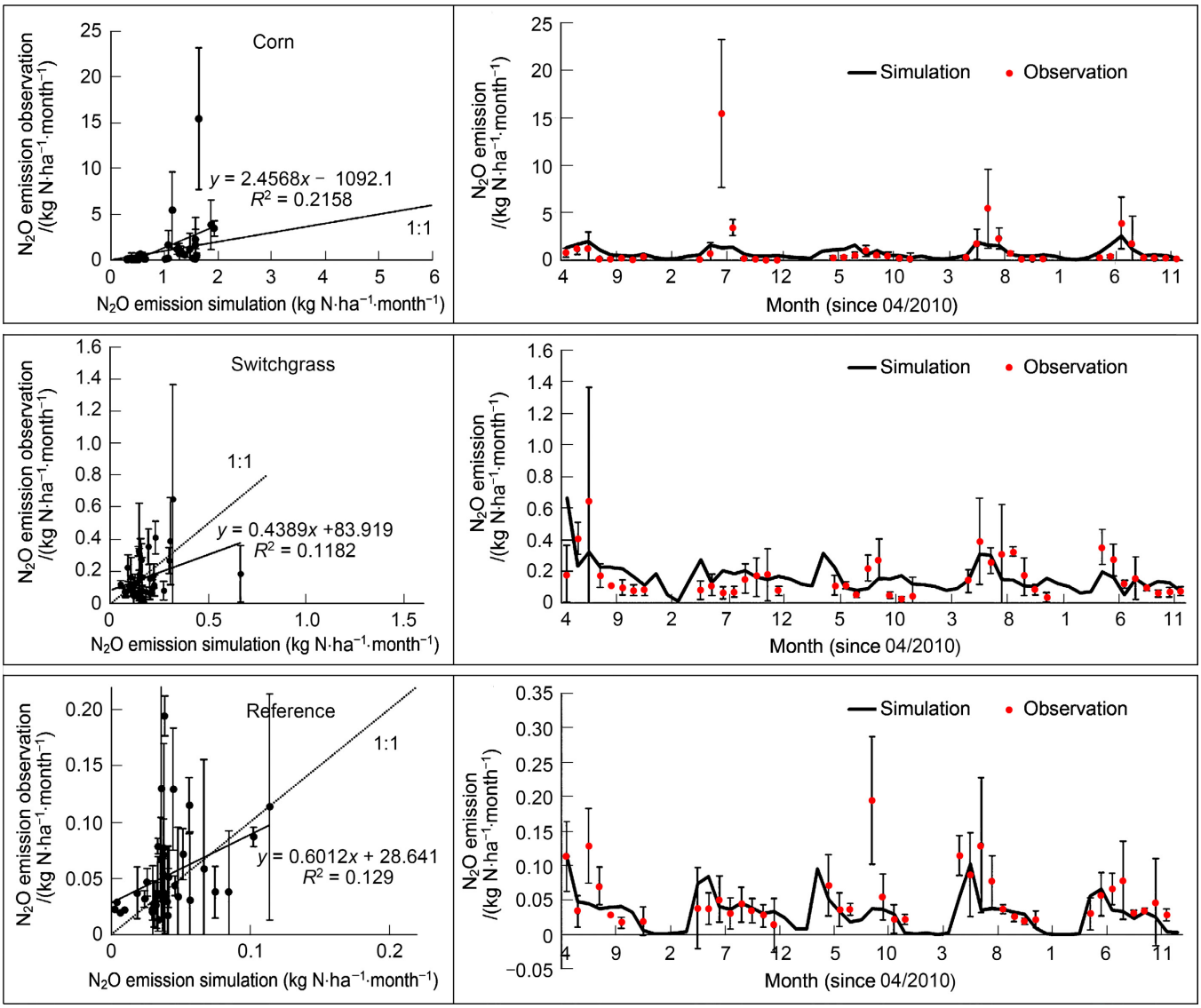

Fig. 4. Comparison of calibrated N_2O estimates with observations at the three sites. Model calibration was conducted manually to optimize parameter values and minimize discrepancies between simulation and observation.

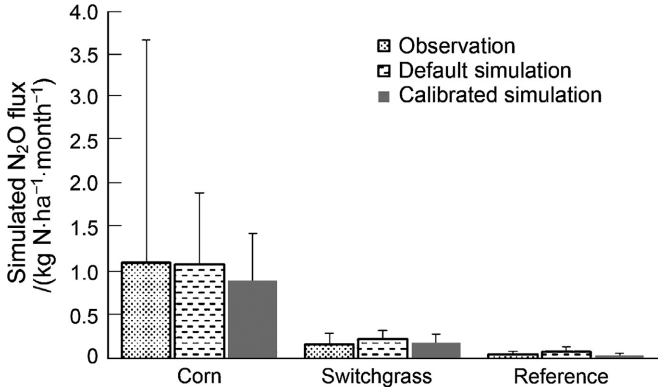

Fig. 5. Comparison of simulated and observed N_2O fluxes across the selected sites. Here, long-term average N_2O fluxes during 2010–2014 at each site were calculated for the comparison.

tool, along with the existing capability of SWAT, to conduct comprehensive assessments of farming impacts on the environment.

Difference in N_2O emissions between managed and unmanaged sites

Our simulations indicate that the corn and switchgrass sites had much higher N_2O emissions than the unmanaged reference site. The difference further confirms the dominant impacts of nitrogen inputs on N_2O emission. Annual average N_2O emissions from the corn site reached 8.48 kg N·ha^{-1}·yr^{-1} during 2009–2014. This emission rate fell within previous observations (approximately 3.29–8.76 kg N·ha^{-1}·yr^{-1}) in the U.S. corn belt (Iqbal et al. 2015), with the emission factor (fraction of N_2O emission to fertilizer use) at the corn site (5.3%) being at the upper end

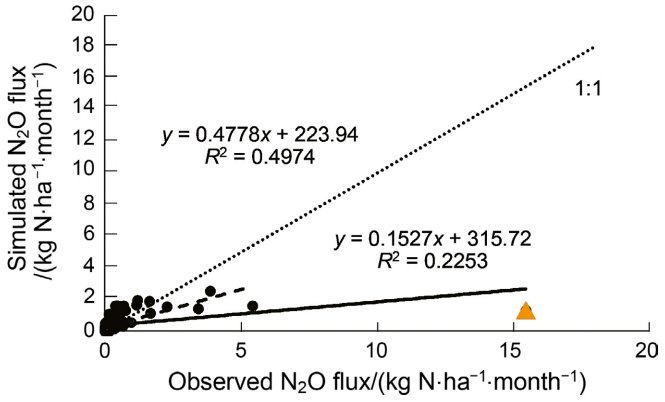

Fig. 6. Scatter plot of simulated and observed monthly N_2O fluxes across the three sites. The orange triangle represents extremely high N_2O emissions observed in June 2011 (note that if the month with extremely high N_2O emissions was excluded in the model-data comparison, the model would explain 49.7% of the variability in N_2O fluxes).

of the range (0.17%–21%) from previous studies (Novoa and Tejeda 2006, Signor et al. 2013). The high emission factor at the corn site may result from the high precipitation in this region (Dobbie et al. 2003).

Investigations of nitrogen cycling in switchgrass cultivation have increased since this species has been identified as a promising cellulosic bioenergy crop (Vogel et al. 2002, Demissie et al. 2012). Previous studies found significant variability in N_2O emissions from switchgrass sites with different fertilizer use rates, soil types, and climate conditions (Wang et al. 2015). Our estimate of 1.96 kg N·ha^{-1}·yr^{-1} at the switchgrass site is consistent with a synthesis (ranging from 1.37 to 2.07 kg N·ha^{-1}·yr^{-1}) across multiple field sites (Oates et al. 2016). We derived a lower emission factor at the switchgrass site (3.3%) than at the corn site (5.3%), which may be explained by the high nitrogen-use efficiency at the switchgrass site (Monti et al. 2012).

For the unmanaged reference site, N_2O emissions reached 0.35 kg N·ha^{-1}·yr^{-1}, which is lower than the average of synthesis data (1.75 kg N·ha^{-1}·yr^{-1}) over more than 200 grass land sites (Kim et al. 2013*a*), indicating that the reference site may have relatively tighter nitrogen cycling. Although the managed sites had much higher emissions than the unmanaged site, their seasonal emission patterns were consistent, with much higher emission rates in summer (May–July) than other seasons, reflecting the fundamental influences of temperature on the seasonality of N_2O emissions (Butterbach-Bahl et al. 2013, Liu et al. 2013).

N_2O emissions in response to climatic changes

Responses of simulated N_2O emissions to changes in precipitation and temperature provide valuable insights into projecting N_2O emissions under a changing climate. All three sites demonstrated positive responses in N_2O emissions to changes in precipitation. Increased soil moisture after rainfall induces elevated emissions mainly through stimulating microbial activities or enhancing the anaerobic conditions (Signor et al. 2013, Gelfand et al. 2016). Historical data indicate that growing-season precipitation has been increasing since the 1980s in most areas of the Midwest United States (Dai et al. 2016). As a result, this changing rainfall pattern may further stimulate N_2O emissions in summer in this region. In contrast, other studies reported that plant growth following elevated rainfalls may deplete the soil inorganic nitrogen pool and thus reduce N_2O emissions (Xu-Ri et al. 2012). Different response rates of N_2O emissions to changes in precipitation at sites with different plant species and management activities, as demonstrated in our analyses, call for further investigations on confounding processes determining N_2O emissions to better predict how future precipitation changes can affect N_2O fluxes.

Model-simulated N_2O fluxes generally increased under higher temperatures across the three sites. Positive responses of N_2O emissions to higher temperatures may be caused by more active microbial activities and increased soil organic matter decomposition (Reth et al. 2005, Signor et al. 2013). Substantial increases at the corn site under the warmer climate scenarios suggested that elevated air temperatures may further enhance N_2O emissions to the atmosphere. Although unmanaged ecosystems contribute much less N_2O emissions than cultivated cropland, enhanced N_2O emissions from the unmanaged site under warming temperatures suggested that the role of unmanaged ecosystems in emitting N_2O should not be ignored under a warming climate (Xu-Ri et al. 2012).

Uncertainties and future work

Although the new modeling tool provided reasonable estimates of N_2O emissions over the three sites, the

Table 2. Sensitivity of N_2O emissions to changes in key parameters.

Parameters	Changes in parameter (%)	Changes in N_2O emissions		
		Corn site (%)	Switchgrass site (%)	Reference site (%)
adj_{fc}	−20	−9.41	−12.19	−12.68
	+20	+9.21	+12.14	+12.69
adj_{wp}	−20	−0.19	−0.38	−0.72
	+20	+0.17	–	+0.72
min_nit	−20	–	–	−0.72
	+20	–	–	+0.02
wfps_adj	−20	+86.79	+18.14	+195.10
	+20	−40.48	−33.65	−3.9
f_{nit_max}	−20	−3.62	+0.18	−0.77
	+20	+2.35	−0.19	+0.53

Notes: adj_{fc} is maximum fraction of N_2O to nitrified N at the field capacity; adj_{wp} is minimum fraction of N_2O to nitrified nitrogen at the wilting point; *min_nit* is minimum nitrate concentration required in a soil layer for trace gas calculation; *wfps_adj* is adjustment on inflection point for water-filled pore space effect on denitrification curve (unitless); f_{nit_max} is maximum fraction of ammonia that is nitrified during nitrification (unitless); "–" indicates changes less than 0.01%.

Table 3. Response of N_2O emissions to changes in climatic factors.

Parameters	Changes in variable	Changes in N_2O emission		
		Corn site (%)	Switchgrass site (%)	Reference site (%)
Precipitation	−20%	−3.66	−3.12	−1.52
	+20%	+1.39	+1.50	+1.44
Temperature	+1°C	+3.69	+1.94	+2.68
	+2°C	+14.36	+0.59	+5.74

Note: Negative signs indicate decreases, whereas positive signs denote increases.

unexplained variability in the observed N_2O fluxes suggests that further improvement is needed to better represent processes regulating N_2O emissions. For example, current model simulation is highly sensitive to parameters such as the adjustment on inflection point for water-filled pore space effect on denitrification curve (*wfps_adj*), which represents soil properties affecting soil diffusivity other than soil water, soil texture, and soil bulk density. Process-based algorithms or spatially explicit datasets are needed to better model underlying mechanisms represented by this parameter to enhance N_2O simulation in the future.

Notably, both nitrification of soil ammonia and denitrification of soil nitrate contribute to N_2O production (Bateman and Baggs 2005). However, field observations at the three sites did not differentiate the relative contributions of each process to total N_2O emission. As a result, N_2O fluxes produced by nitrification and denitrification were lumped together to calibrate and evaluate simulated total N_2O fluxes from soil columns. As a result, future model improvement should focus on the model simulation of the individual processes in N_2O production, the soil inorganic nitrogen stocks, etc., to further strengthen the model's capability in modeling N_2O fluxes.

In addition, our analysis indicated that extremely high N_2O fluxes observed after fertilizer use dramatically affected model performances. Therefore, more frequent observations, in particular following fertilizer use, are needed to improve model performance by incorporating observational information through calibration.

Although manual calibration of the parameters directly controlling N_2O production improved model performances, more comprehensive parameter optimization is needed to further enhance model simulations. Parameter sensitivity analysis in this study identified impacts of individual parameters on model estimates of N_2O emissions. However, interactions among these parameters may jointly affect model responses (Kim et al. 2013*b*). As a result, further analysis targeting the interplay among multiple parameters should be conducted in the future. In addition, calibration of parameters that indirectly regulate N_2O production, such as carbon-to-nitrogen ratio for structural litter, leaching coefficient of soil nitrogen, and water limitation coefficient on nitrification, together with the parameters identified in this study, would improve model representation of seasonal variability of N_2O emissions (Rafique et al. 2013).

Conclusions

As a watershed-scale model, SWAT has been widely used to evaluate impacts of agricultural activities on the quality of the aquatic ecosystems (Gassman et al. 2007). However, N_2O emissions were not included in previous SWAT modeling efforts, limiting its use for assessing and identifying best agriculture management practices under climate change. Here, we integrated DayCent's N_2O emission module with the existing crop growth, hydrology, and biogeochemical processes in SWAT, and achieved a new tool (SWAT-N_2O) that reasonably captured the magnitude and seasonality of N_2O emissions from three diverse agricultural systems with different management intensities. Modeled N_2O emission responses to climate change scenarios demonstrate that N_2O emissions may increase under a warmer and wetter climate. Overall, the model development and application efforts enhanced SWAT to represent N_2O emissions as a dimension in assessing sustainability of agricultural ecosystems and to explore climate-smart agricultural solutions under a changing climate.

Acknowledgments

This work was funded by the DOE Great Lakes Bioenergy Research Center (DOE BER Office of Science DE-FC02-07ER64494, DOE BER Office of Science KP1601050, DOE EERE OBP 20469-19145), the NASA New Investigator Award (NNH13ZDA001N) and Terrestrial Ecology Program (NNH12AU03I and NNX17AE66G), and NSF INFEWS (1639327).

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Supporting Information

Additional supporting information may be found in the online version of this article at http://onlinelibrary.wiley.com/doi/10.1002/ehs2.1259/suppinfo

Supplementary Material

1. Calculation of diffusivity

$$dD0_{fc} = \frac{tp8}{10^7} + tp7 \times tp6$$

$$tp8 = \frac{\text{tp1} \times \text{tp3} \times \text{tp4} \times (\text{tp5} - \text{tp6})}{1.0\text{E} - 6 + (\text{tp1} \times \text{tp3} \times \text{tp4}) + \text{tp5} - \text{tp6}} \times 10^7$$

$$\text{tp1} = (1 - \frac{pfc}{100})^2$$

$$pfc = \frac{wfps}{A} \times porosity$$

$$\text{tp2} = \frac{A - \frac{pfc}{100} \times A}{A + 1 - porosity}$$

$$\text{tp3} = \text{tp2}^{0.5 \times tp2 + 1.16}$$

$$\text{tp4} = 1 - (porosity - A)^{0.5 \times (porosity - A) + 1.16}$$

$$\text{tp5} = porosity - A - theta\_P$$

$$theta\_P = \frac{pfc}{100} \times A - A$$

$$\text{tp6} = \text{tp5}^{0.5 \times tp5 + 1.16}$$

$$\text{tp7} = (1 - \text{swp})^2$$

$$\text{swp} = \frac{theta\_P}{porosity - A}$$

where $dD0_{fc}$ is normalized soil diffusivity (unitless); $tp1 - tp8$ are intermediate variables used to calculate diffusivity (unitless); pfc is soil water content expressed as a percent of field capacity (%); $porosity$ is fraction of soil bed volume occupied by pore space (unitless); $theta\_P$ is volume of water per unit bed volume contained in inter-aggregate pore space (unitless); A is

fraction of soil bed volume occupied by field capacity (unitless); Swp is fractional liquid saturation of total pore volume (unitless); $swcfrac$ is volumetric soil water content (unitless).