Simulating N₂O emissions under different tillage systems of irrigated corn using RZ-SHAW model

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ABSTRACT

Nitrous oxide (N₂O) is a potent greenhouse gas (GHG), and agriculture is a global source of N₂O emissions from soil fertility management. Yet emissions vary by agronomic practices and environmental factors that govern soil moisture and temperature. Ecosystem models are important tools to estimate N₂O emissions by accounting for such variables, and models can strengthen field research. The objective of this study was to test RZ-SHAW predictions of crop production and N₂O emissions from conventional till (CT) and no-till (NT) systems at high (HN) rate and low nitrogen input (LN) treatments in an irrigated corn (*Zea mays* L.) field in Colorado from 2003 to 2006 growing seasons. The model was calibrated using the HN-CT, and other treatments were used as validations. Additionally, the SHAW model was run in conjunction with RZWQM2 to account for differences in soil surface temperatures. Simulated crop yields were within 0.7 and 0.9% of measured yield for HN-NT and CT treatments, and 32 and 3% of measured yield for LN-NT and CT treatments, respectively. Spring soil temperatures were cooler by 2 °C in NT compared to CT, and were correctly simulated using RZ-SHAW coupled model. RZ-SHAW simulated N₂O emissions were slightly under predicted by 0.10 (1.5%) and 0.56 (7.1%) kg N ha^{-1} for HN-NT and HN-CT treatments, respectively. Results for LN treatments showed larger differences in simulated N₂O emissions and were over predicted by 0.11 (16%) kg N ha^{-1} in NT and under predicted by 0.29 (29%) g N ha^{-1} day^{-1} in CT. Annual emissions were in close agreement, with observed and simulated showing 12 and 10% lower N₂O emissions from HN-NT than HN-CT, respectively. Cooler surface soil temperature and higher soil water content in the HN-NT treatment caused slower breakdown of crop residue and slightly more denitrification than HN-CT, resulting in lower N₂O emissions in HN-NT. This is the first test of the newly added GHG component in RZ-SHAW under no-till management, and results suggest with some improvements the model could be applied to quantify N₂O emissions from different management practices.

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1. Introduction

Nitrous oxide (N₂O) is a greenhouse gas (GHG) with impending environmental effects because of its persistence in the atmosphere, high radiative feedback, unchecked emissions, and lack of terrestrial sinks (Ravishankara et al., 2009). Agricultural is a global source of N₂O emissions through the use of fertilizer and manure applications (Cavigelli et al., 2012). N₂O is produced as one of the intermediate N gas byproducts due to the incomplete pathway of nitrification and denitrification (Parton et al., 2001). Conventional farming systems are dependent on synthetic N fertilizer for economic yield return, therefore, as global population rises and food demand increases emissions are expected to intensify (Keeney and Hatfield, 2008; Reay et al., 2012; Bouwman et al., 2013). One of the best predictors of N₂O emissions is N fertilizer rate (Miller et al., 2010) which increases the availability of N for microbial transformation (Bouwman et al., 1993). Yet, emissions

vary by crop type, management, N fertilizer type and application timing, tillage, and irrigation practices (Mosier et al., 2006; Dobbie and Smith, 2003; Parkin and Kaspar, 2006). Emissions also vary by year because climate factors play a significant role in regulating soil moisture and temperature (Lesschen et al., 2011). Therefore strategies to mitigate N_2O emissions are complex and results can be difficult to predict.

Consequently, it is critical for process based models to reflect an appropriate response in soil N_2O emissions caused by environmental factors and management practices (Metivier et al., 2009; Wang et al., 2012; Fang et al., 2015). In general, process based models provide a systematic approach to understanding field research based on specific management (Ahuja and Hatfield, 2007) and allow comprehensive evaluation of multiple ecosystem processes (Zhang et al., 2013). Simulating the complexity of the primary ecological drivers affecting the soil N cycle and its interaction with management, have often yielded mixed results from ecosystem models regarding N_2O emissions (Del Grosso et al., 2008; David et al., 2009; Bessou et al., 2010). Therefore, continuously testing and updating the current knowledge of N_2O emissions kinetics is critical to improving models.

Root Zone Water Quality Model 2 (RZWQM2) is a comprehensive ecosystem model that simulates soil water, temperature and C/N dynamics as influenced by various agronomic management practices (Ahuja et al., 2000). RZWQM2 has been extensively applied to better understand the effects of soil water and N fertilizer management on crop yield and their interactions in the environment (Ma et al., 2007; Malone et al., 2007; Fang et al., 2008, 2010, 2012). Detailed input data for weather, soil physical, chemical and hydraulic information, and agronomic management are required to run the model (Ma et al., 2011; Malone et al., 2011), and Parameter Estimation Software (PEST) is included to support efficient user calibration (Ma et al., 2012b). Recently, to better quantify effects of alternative management practices and environmental impacts on nitrification and denitrification, Fang et al. (2015) modified RZWQM2 to simulate N_2O emissions. Those

authors used algorithms for nitrification and denitrification as a function of soil water, temperature and soil N levels (Parton et al., 2001; Khalil et al., 2005; Bessou et al., 2010). However, their study was focused on conventional tillage only and the detailed surface energy balance component (simultaneous heat and water (SHAW)) was not used. The RZ-SHAW hybrid model adds the capability of simulating the effects of agriculture management on the surface energy balance (Flerchinger et al., 2000), and has shown improvement over the original RZWQM model in simulating the effects of crop residue on soil moisture and soil temperature (Kozak et al., 2007; Ma et al., 2012a).

No-till is a common agronomic soil conservation practice that reduces erosion and mitigates energy consumption in crop production (Halvorson et al., 2006). No-till management is a recognized and feasible soil conservation method for intensively managed systems such as corn (*Zea mays* L.) (Halvorson and Jantalia, 2011). There have been mixed findings however as to whether no-till reduces N_2O emissions from cropping systems (Mosier et al., 2006; Liu et al., 2005). Tillage management affects soil temperature and soil water content and finally crop yield (Halvorson et al., 2008; Halvorson and Jantalia, 2011). Correctly predicting effects of tillage caused by changes in crop residue and soil hydraulic properties should improve model results for soil temperature (Ma et al., 2012a) and soil water content (Wang et al., 2010), and in turn improve simulated N_2O emissions. Fang et al. (2014) showed that the RZ-SHAW was reasonable for simulating soil water content, soil temperature, evapotranspiration, surface energy balance as well as crop growth under conventional tillage conditions. The influence of no-till management on soil temperature and soil water content from surface residue cover and soil hydraulic properties has not been evaluated using RZ-SHAW (Ahuja et al., 2000).

The objective of this study was to test RZ-SHAW in predicting N_2O emissions from no-tillage and conventional tillage management at two fertilizer application rates from an irrigated continuous corn (*Zea mays* L.) system in Colorado. This is a
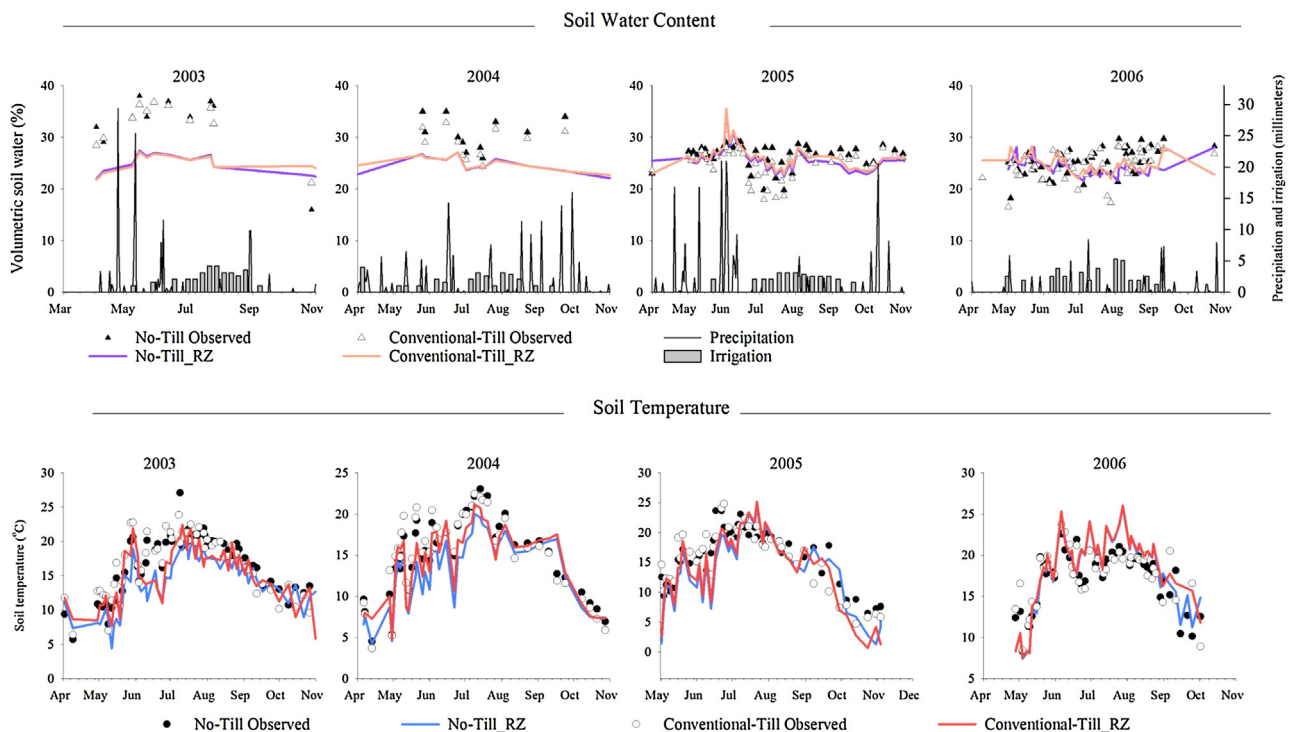
Fig. 1. Observed and RZ-SHAW simulated soil water ($cm^3\ cm^{-3}$) (0–5 cm) and soil temperature (0–5 cm) during the 2003–2006 study period, along with millimeters of precipitation and irrigation water applications to field plots.

continuation of the study by Fang et al. (2015) to include effects of no-till management on N₂O emissions and surface soil temperatures. Different from Fang et al. (2015), we used the RZ-SHAW version for both till and no-till, in which surface energy balance was used to improve soil surface temperature estimates, rather than assuming surface soil temperature equals air temperature.

2. Materials and methods

2.1. Field experiment

The experiment was conducted in clay loam soil (fine-loamy mixed, superactive mesic Aridic Haplustalfs) at the Agriculture Research Development and Education Center (ARDEC) (40°39′6″N. 104°59′57″S.; 1555 m above sea level) near Fort Collins, Colorado (Halvorson et al., 2006). The annual precipitation was 21.8 cm, 24.2 cm, 29.6 cm, and 11.7 cm in 2003, 2004, 2005, and 2006. The soil had a pH of 7.71, organic matter content of 21 g kg⁻¹, and a clay and silt contents of 33% and 27%, respectively (Halvorson et al., 2006). To evaluate management effects of conventional till (CT), no-till (NT) and nitrogen fertilizer rates in a continuous corn cropping system a study was established in 1999 (Halvorson et al., 2006). Prior to plot establishment the field was in conventionally tilled continuous corn for 6 years. In the CT corn system corn stalks were shredded in the fall and incorporated into the soil using a tandem disk; after disking, soil were turned using a moldboard plow at a depth of 25–30 cm. To prepare a seedbed in the spring, two operations of roller harrowing and two operations of land-leveling was conducted prior to land cultivation in the CT system. In the NT system, to facilitate planting, the corn planter was equipped with trash whippers to manage residue, otherwise corn was planted directly into the previous year's corn stalks. Corn was planted with 76 cm row spacing. Corn hybrids were changed each year based on hybrid availability, herbicide resistance and new yield potentials, but most hybrids had a 92–94 day relative maturity.

Four N fertilizer rates were designed with three replicates under the conventional and no-till systems. For this analysis however only the low N (0 kg N ha⁻¹) and high N fertilizer rates were evaluated. In 2003 and 2004, the high N rate of 224 kg N ha⁻¹ in the form of urea ammonium nitrate (UAN) was injected to the top 5 cm of the soil profile prior to corn planting in late April of each year. In 2005 and 2006 a total of 246 kg N ha⁻¹ was applied in a split application. In 2005, 123 kg N ha⁻¹ was applied in a subsurface banded as UAN on 25 Apr., and 123 kg N ha⁻¹ of polymer-coated urea (PCU) was broadcast on 9 June. In 2006, the PCU was broadcast first on 17 May and urea was surface-band on 12 June at a rate of 123 kg N ha⁻¹. A lateral moving sprinkler system was used to apply irrigation water to CT and NT on a weekly basis during the corn growing season. Total irrigation amounts were 41.6 cm, 36.21 cm, 38.77 cm, and 40.28 cm in 2003, 2004, 2005, and 2006, respectively. Precipitation and irrigation water applications for each year are presented in Fig. 1.

In September of each year corn biomass was determined by hand harvesting 15 whole corn plants from a specified area of each plot and plants were separated into grains, cobs, and stover to determine total mass. Corn grain yield was determined in late October by hand harvesting ears from an 11.6 m² area of each plot. Corn ears were shelled to determine grain and cob weight. Prior to planting in the spring, residue cover was estimated using the transect line method. Grain and crop residue were ground to pass a 150 μm sieve for N analysis and analyzed using a Carlo Era C/N analyzer (Haak Buchler instruments, Inc., Saddle Brook, NJ). See Halvorson et al. (2006) for more specifics of the field study.

Measurements of the soil-atmosphere exchange of N₂O emissions were made throughout the corn growing seasons (April–Ocotober) following the same procedures as Mosier et al. (2006), and were generally made two to three times per week using the vented non-steady state closed chambers technique (Hutchinson and Mosier, 1981; Livingston and Hutchinson, 1995). Rectangular chamber lids were fit onto water filled anchors that were set into the top 10 cm of soil, and gas samples inside the chamber were collected by syringe at time interval of 0-, 15- and 30- minutes. Upon trace gas collection, samples were injected into vacuum sealed 25 ml exetainers, and analyzed by gas chromatography. Nitrous oxide concentrations were analyzed using a fully automated gas chromatograph equipped with an electron capture detector (Varian 3800; Varian Inc., Palo Alto, Cali). Nitrous oxide flux rates were calculated based on linear or non-linear concentration increases in chamber head space (Hutchinson and Mosier, 1981; Livingston and Hutchinson, 1995). To estimate annual N₂O emission, linear interpolations between sampling days were used as flux estimates for non-sampling days. Further detailed information regarding experimental design, trace gas measurements, and calculations can be found in Halvorson et al. (2008, 2010).

Surface soil water content and temperature measurements coincided with soil trace gas measurements and were measured using dielectric soil probes (Decagon Devices, Inc., Pullman WA., USA). Soil mineral N was measured from each treatment plot prior to planting in the spring and after harvest in the fall of each year from 2003 to 2006 and analyzed using a continuous flow analyzer (LACHAT Quick-Chem FIA + 8000 Series, Lachat Instrumentation) after extraction with 1 M KCl. One soil core was taken from the near center of each plot before planting and after harvest in the 0–180 cm of the soil profile each year from 2003 to 2006 for determination of gravimetric soil water content by oven drying soil subsamples at 105 °C.

2.2. N₂ emission algorithms

Prior to modifications of the new RZWQM GHG submodel made by Fang et al. (2015), nitrification and denitrification were simulated using a zero and first order kinetics, respectively (Ma et al., 2001). In order to comprehensively test the existing N₂O algorithms Fang et al. (2015) modified RZWQM sub model to estimate N₂O emissions based on soil water content, soil temperature, and soil N content. The algorithms presented below are currently being tested in RZWQM and are partially based on the general nitrification and denitrification models developed for DAYCENT as described by Parton et al. (2001) and Del Grosso et al. (2001). Specifically, the N₂O emission ($N_2O_{\_nit}$) during nitrification (R_{nit}) is from the DAYCENT model (using a fixed proportion of nitrification to estimate N₂O emissions) and modified by a soil water factor (F_{SW_Nit}) of the oxygen availability effect on N₂O emission during nitrification (Khalil et al., 2005) as the following:

$$N_2O_{\_nit} = Fr_{N_2O\_Nit} \times F_{SW\_Nit} \times R_{nit} \tag{1}$$

$$F_{SW\_Nit} = \frac{0.4 \times WFPS - 1.04}{WFPS - 1.04} \tag{2}$$

where $Fr_{N_2O\_Nit}$ is a proportion of nitrification for N₂O emissions, and a value of 0.02 was used as default in DAYCENT model (Parton et al., 2001; Del Grosso et al., 2001). WFPS is water filled pore space.

N₂O emissions ($N_2O_{\_den}$) from denitrification (R_{den}) is followed according to the DAYCENT model (Del Grosso et al., 2000) where ratios of N₂ to N₂O and NO to N₂O are estimated and modified based on soil nitrate-N content, soil respiration, and water filled

pore space (WFPS) as the following.

$$N_2O_{\_den} = Fr_{N_2O\_Den} \times R_{den} \tag{3}$$

$$Fr_{N_2O\_Den} = \frac{1}{1 + R_{NO\_N_2O} + R_{N_2\_N_2O}} \tag{4}$$

$$R_{NO\_N_2O} = 4 + \frac{9 \times \tan^{-1}(0.75 \times \pi \times (10 \times D - 1.86))}{\pi} \tag{5}$$

$$R_{N_2\_N_2O} = \max\left(0.16k1, k1 \times e^{\frac{-0.8[NO3]}{[co2]}}\right) \\ \times \max(0.1, 0.015 \times WFPS \times 100 - 0.32) \tag{6}$$

$$k1 = \max(1.5, 38.4 - 350 \times D) \tag{7}$$

where $Fr_{N_2O\_Den}$ is the fraction of denitrification for N_2O emissions; $R_{NO\_N_2O}$ is the ratio of NO to N_2O; $R_{N_2\_N_2O}$ is the ratio of N_2 to N_2O; $[NO_3]$ is soil nitrate-N content; $[CO2]$ is CO_2 concentration; D is O_2 diffusivity in soil (Davidson and Trumbore, 1995).

Since the above described N_2O emission simulation processes from DAYCENT model do not account for N_2O diffusion across soil depth, another modification is a diffusion factor ($F_{depth\_N_2O}$) of soil depth (depth, m) added to N_2O emission from both nitrification and denitrification based on Chatskikh et al. (2005) as following:

$$F_{depth\_N_2O} = \max\left(0, \min\left(1, 1.0008 - 0.0343 \times depth - 3.186 \times depth^2\right)\right) \tag{8}$$

Based on the Eq. (3), N_2O from soil depth below 60 cm has no contribution to measured N_2O on the surface, which can be applicable in simulating N_2O emissions from deep soil layer in response to the irrigation or N fertilizer application methods (such as N application by injection and or subsurface irrigation).

2.3. Model input and SHAW model description

The simulation started in 1999 to initialize soil C and N and hydrology prior to the calibration. The calibration and testing period was from 2003 to 2006 and using the measured data of soil water, soil temperature, soil nitrate-N, crop yield, above ground biomass, and crop N uptake from the HN-CT treatment, while other N rate treatments in the CT system were used for validation as described by Fang et al. (2015). For this study, the calibrated RZWQM model from Fang et al. (2015) was used to further validate the experimental results from the high N (HN) and low nitrogen input (LN) treatments of the no-till system during the same measurement period of 2003–2006. Model input was based on the two corn systems described in the aforementioned field experiment. The only difference in management was tillage practices, in which no-till cropping systems were simulated with surface residue at the time of planting. Additionally, the SHAW model was run in conjunction with RZWQM2 to account for differences in soil surface temperatures due to surface residue cover (Ma et al., 2012a).

The SHAW model was originally developed by Flerchinger et al. (2000, 2009) and was incorporated into RZWQM to improve surface energy balance simulation (Li et al., 2012; Ma et al., 2012a; Fang et al., 2014). RZWQM provides SHAW soil water content, root distribution, soil evaporation, soil transpiration, leaf area index, and plant height at each time step. Then SHAW feeds back to RZWQM with soil ice content, updated soil water content due to ice and freezing, and soil temperature (Fang et al., 2014). Soil evaporation (AE) supplied by the RZWQM is used in SHAW to compute the energy balance of the surface soil layer by forcing water vapor flux from the soil surface, and therefore latent heat flux, to equal the soil evaporation. Soil heat flow and temperature in the soil matrix, considering convective heat transfer by liquid and latent heat transfer by vapor for freezing soil is given by

$$C_s\frac{\partial T}{\partial t} - \rho_i L_f\frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z}\left[K_{t(s)}\frac{\partial T}{\partial z}\right] - \rho_l c_l\frac{\partial q_l T}{\partial z} - L_v\left(\frac{\partial q_v}{\partial z} + \frac{\partial \rho_v}{\partial t}\right) \tag{9}$$

where C_s and T are volumetric heat capacity ($J\,kg^{-1}\,K^{-1}$) and temperature (°C) of the soil, ρ_i is density of ice ($kg\,m^{-3}$), θ_i is volumetric ice content ($m^3\,m^{-3}$), $K_{t(s)}$ is soil thermal conductivity ($W\,m^{-1}\,K^{-1}$), ρ_l is density of water, c_l is specific heat capacity of water ($J\,kg^{-1}\,K^{-1}$), q_l is liquid water flux ($m\,s^{-1}$), q_v is water vapor flux ($kg\,m^{-2}\,s^{-1}$), L_f is latent heat of fusion (335,000 J/kg) and ρ_v is vapor density ($kg\,m^{-3}$) within the soil. The soil thermal conductivity and heat capacity are quantified using the theory of de Vries (1963). SHAW also uses a Newton-Raphson algorithm (Campbell, 1985) to solve finite difference expressions of the energy balance equation for soil temperature profiles. Soil surface temperature is solved through this iteration process by balancing radiation, sensible and latent heat fluxes from above with the soil heat flux (G) into the soil. G is calculated by rearranging Eq. (9) as the sum of gradient and storage terms for a soil slab thickness (Δz_s, m) as follows

$$G = \left[\frac{K_{s(t)}}{\Delta z_s} + c_l q_l\right]\left(T_{s(t)} - \hat{T}_{z(t)}\right)$$

$$-\frac{\Delta z_s}{2\Delta t}\left[C_s\left(T_{s(t)} - T_{s(t-\Delta t)}\right) - \rho_i L_f\left(\theta_{i(t)} - \theta_{i(t-\Delta t)}\right)\right] + L_v q_v \tag{10}$$

where Δt is time increment (s), $T_{s(t)}$ is surface soil temperature at time t (°C), $T_{s(t-\Delta t)}$ is previous surface soil temperature at time t-Δt (°C), $\hat{T}_{z(t)}$ is soil temperature expected at soil slab lower boundary z at time t (°C). Other information on RZ-SHAW can be found in Fang et al. (2014).

2.4. Evaluation criteria

RZ-SHAW performance of simulated crop yield, biomass, crop N uptake, daily water content, soil temperature, and seasonal soil nitrate (NO_3-N) was evaluated using the following statistics: root mean square error (RMSE), mean difference (MD), coefficient of determination (r^2), and Nash-Sutcliffe model efficiency (NSME). The respective equations are shown below:

$$RMSE = \sqrt{1/N\sum_{i=1}^{N}Pi - Oi^2} \tag{11},$$

$$MD = \frac{\sum_{i=1}^{N}(Pi - Oi)}{N} \tag{12},$$

$$r^2 = 1 - \frac{\sum_{i=1}^{N}(Pi - Oi)^2}{\sum_{i=1}^{N}(Pi - Oi)^2 + \sum_{i=1}^{N}(Pi - Oa)^2} \tag{13},$$

$$NSME = \frac{\sum_{i=1}^{N}(Pi - Oi)^2}{\sum_{i=1}^{N}(Oi - Oa)^2} \tag{14}$$

Where Pi and Oi are paired simulated and observed results, Oa is the average of observed values over the 2003–2006 measurement periods, and N is the number of data pairs. The NSME was calculated to statistically compare observed and simulated cumulative N_2O emissions from 2003 to 2006. NSME is a statistical calculation used to normalize residual variance between observed and simulated data and evaluate how well the data fit on a 1:1 line comparison (Moriasi et al., 2007). Soil water content, soil temperature and N_2O emissions were averaged over the four year (2003–2006) during the early (April-June), mid (July-August), and late (September–October) growing season, and correlations (R^2) between observed and simulated results are used to compared differences.

3. Results and discussion

3.1. Tillage effects on yield and N uptake

Simulated crop yield during the four year simulation period (2003–2006) was in good agreement with the measured data for all HN and LN tillage treatments, with mean difference (MD) values of $<0.9\,Mg\,ha^{-1}$, root mean squared errors (RMSE) of $<1.2\,Mg\,ha^{-1}$, and Nash-Sutcliffe Model Efficiency (NMSE) values of >0.4 (Table 1). Simulated aboveground biomass closely matched measured data as well, with corresponding to RMSE values of 1.7, 1.6, 1.5, and 1.3 Mg ha^{-1} for HN-NT, HN-CT, LN-NT, and LN-Ct treatments, respectively (Table 1). Overall, yield and biomass were closely simulated to the measured data among the various tillage treatments, especially in that predicted crop production was slightly lower in the NT treatments compared to CT treatments. Grain N content was over predicted for all tillage treatments, which corresponded to negative NMSE values (Table 1). Thorp et al. (2008) also reported an over prediction of grain N uptake by15 and 40% using RZWQM. Similar to grain N content, RZ-SHAW simulated plant N uptake was also over predicted, but was most exaggerated in the HN-NT and HN- CT treatments, with RMSE values of 53.9 and 43.9 kg N ha^{-1} and negative NMSE values of 3.7 and 3.5, respectively (Table 1). Fang et al. (unpublished) evaluated different grain N concentrations algorithms for modern hybrid corn which may improve comparisons between measured and modeled data.

3.2. Soil water, temperature, and nitrate

Although irrigation management was similar between the NT and CT treatments, tillage practices created differences in soil water content and soil temperature. Soil water content (0–10 cm) and soil temperature (0–5 cm) were similar among the N treatments within the two tillage systems, and were averaged across N treatments. In general, RZ-SHAW responded to field conditions in the NT and CT systems, but simulated soil water content was under predicted during 2003 and 2004 (Fig. 1). There was abnormally high soil water content (>0.36) measured in the field during 2003 and 2004 caused by high precipitation events of >4.5 cm during the early growing season (Liu et al., 2005; Halvorson et al., 2014). Simulated field capacity in the 0–10 cm layer of the soil is 0.334 in the calibrated model, but simulated soil water content ranged between 0.24 and 0.27 during the early growing seasons of 2003 and 2004 (Fig. 1), suggesting that movement of water through the soil profile was over predicted. The 1:1 comparison in Fig. 2a, demonstrates the tendency of the model to under predict surface soil water content (0–10 cm) on a seasonal basis, especially in the NT treatment, and illustrates the slightly drier soil conditions measured for the CT treatment (Fig. 2b).

Averaged over the four year study period surface soil water content (0–10 cm) was under predicted in the NT treatments, with residual mean differences (MD) of $-0.02\,cm^3\,cm^{-3}$ and RMSE values of 0.05 cm^3 cm^{-3} (Table 2). Root mean square errors (RMSE) values from 0.02 to 0.05 cm^3 cm^{-3} have been used for simulated soil water content in model tests using RZWQM (Cameira et al., 2005). By excluding surface water content during the early 2003 growing season NMSE values are slightly improved from -0.14 to -0.03. Our results are similar to Fang et al. (2015), who also reported near zero NMSE values of 0.09 and 0.06 for soil water content in the calibration and validation CT treatments, respectively. Predicted soil water content for 2003–2006 was closer to measurements from CT treatments, with a MD and RMSE values of -0.006 and 0.02 cm^3 cm^{-3} (Table 2).

By excluding the high profile soil water storage of 57 cm measured during spring of 2003, statistical comparisons between observed and simulated water storage was improved from an initial NMSE value of -0.34 (shown in Table 2) to 0.12. Averaged over the four year study period (2003–2006), water storage in the 0–180 cm soil profile was under predicted for NT treatment by nearly 4%, with MD and RMSE values of -1.8 cm and 2.8 cm, respectively (Table 2). Fang et al. (2010) also reported a disagreement in stored soil water under wet soil conditions, with a RMSE value of 5.4 cm, a 15% difference between observed and predicted profile soil water from a winter wheat maize double cropping system in Northern China. There was a slight improvement (2–5%) using RZ-SHAW coupled model for simulated soil water storage compared to the initial analysis of the conventional

Table 1
Statistical (MD, mean difference; RMSE, root mean square error) results between observed and RZ-SHAW simulated (RZ)crop growth variable of yield (Mg ha^{-1}), biomass (Mg ha^{-1}), grain N content (kg N ha^{-1}) and Plant N uptake (kg N ha^{-1}) for no-till (NT) and conventional-till (CT) high N rate (HN) rate and low N input (LN) from 2003 to 2006.

Tillage	N Rate	Yield Mg ha^{-1}						Biomass Mg ha^{-1}						Grain N kg N ha^{-1}						Plant N kg N ha^{-1}					
		Obs	RZ	MD	RMSE	r^2	NMSE	Obs	RZ	MD	RMSE	r^2	NMSE	Obs	RZ	MD	RMSE	r^2	NMSE	Obs	RZ	MD	RMSE	r^2	NMSE
NT	HN	9.1	9.2	0.1	0.9	0.3	0.5	17.5	16.8	−0.7	1.7	0.6	−0.9	125	164	39.9	43	0.5	−4.3	186	224	33.6	53.9	0.3	−3.7
	LN	4.2	5.5	0.9	1.2	0.5	0.6	10.0	11.1	1.7	1.5	0.3	−0.6	41	51	10.1	18	0.2	−3.7	63	73	10.0	16.0	0.3	−0.6
CT	HN	10.1	10.2	0.4	0.9	0.3	0.4	17.3	18.3	0.9	1.6	0.6	−0.2	130	172	42.6	63	0.6	−2.0	197	233	42.2	43.9	0.3	−3.5
	LN	5.5	5.7	0.2	0.4	0.5	0.7	11.3	11.6	0.3	1.3	0.8	0.7	53	57	3.6	14	0.2	−2.7	77	81	4.4	9.3	0.4	0.04

Table 2
Statistical (MD, mean difference; RMSE, root mean square error; NSME, Nash-Sutcliffe model efficiency; r^2, coefficient of determination) results between observed and RZ-SHAW simulated soil water content at 10 cm, soil temperature at 5 cm, and profile soil water content in the 180 cm for no-till and conventional-till from 2003 to 2006.

Variable	Data Number	Depth (cm)	Obs	RZ	MD	RMSE	NSME	r^2	Obs	RZ	MD	RMSE	NSME	r^2
			No-Till						Conventional-Till					
Soil water content (cm^{-3} cm^{-3})	236	10	0.27	0.25	−0.02	0.04	−0.14	0.31	0.26	0.25	−0.006	0.04	−0.02	0.21
Soil temperature (°C)	402	5	16.0	14.6	−1.4	3.12	0.54	0.75	16.3	15.4	−0.81	2.8	0.64	0.77
Profile soil water (cΔm)	16	180	54.4	52.6	−1.8	3.3	−0.34	0.33	51.8	52.5	0.45	1.8	0.05	0.49
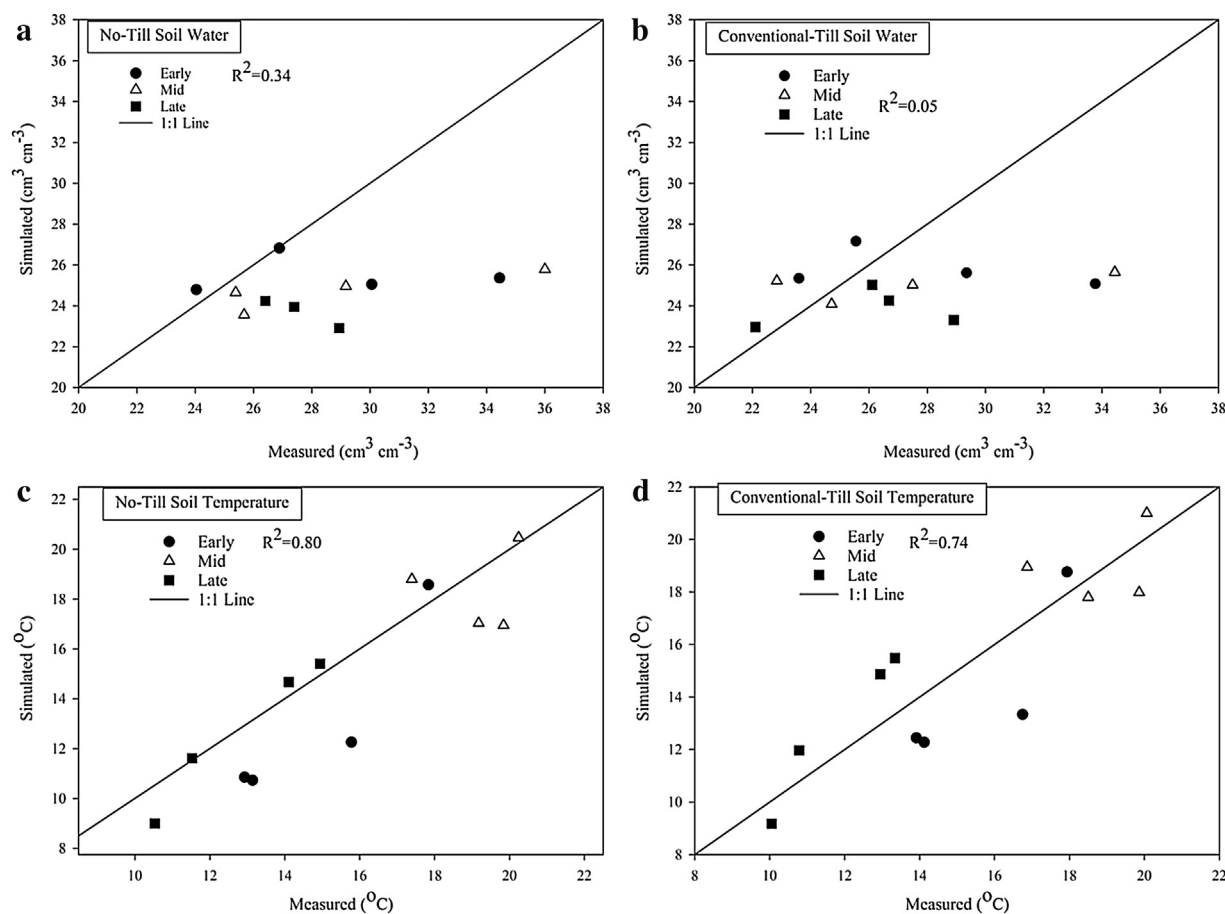
Fig. 2. Observed and simulated simulated soil water content (cm^3 cm^{-3}) in the 0–10 cm soil profile (a and b), and soil temperatures (degrees Celsius) in the 0–5 cm soil profile (c and d) for no-till and conventional-till treatments during the early (April–June), mid (July–August), and late (September–October) growing season of 2003–2006.

tillage system by Fang et al. (2015), which lowered MD and RMSE values of −0.07 cm and 1.2 cm, respectively (Table 2).

In contrast to soil water, predicted soil temperature was in better agreement with the observed data for both tillage systems (Fig. 2c, d). The greater surface cover provided by crop residue in the NT system typically retained 1–2 °C cooler soil temperatures in the early corn growing season and slightly warmer temperatures during the late season (Liu et al., 2005; Halvorson et al., 2006, 2008). Residue insulation effects on soil temperature from no-till management causes differences in seasonal soil temperature regimes compared to conventional tillage (Hayhoe et al., 1996; Dao, 1998; Halvorson et al., 2008). However, there were a few notable discrepancies between observed and simulated data. For example, NT soil temperature was under predicted during the early and mid-growing season of 2004 by around 2 °C, but over predicted by 2 °C for both tillage systems during the mid-2006 growing season (Fig. 1). Observed and simulated soil temperature had RMSE

values of 3.1 °C and 2.8 °C and MD values of −1.4 and −0.9 °C for NT and CT system, respectively (Table 2). Simulated soil temperature was improved in the CT treatment using the RZ-SHAW coupled model compared to Fang et al. (2015) who reported RMSE and MD values of 3.6 and −2.0, respectively. Closer simulation of soil temperature was accomplished using RZ-SHAW because air temperature is not assumed to be equivalent to the soil boundary layer. Furthermore, RZ-SHAW correctly predicted seasonal differences in soil temperature between NT and CT systems. However the insulating effect on soil temperature from surface residue during early (April–June) growing season was over predicted for three of the four years in NT treatments, with simulated soil temperature being 1.0–1.8 °C under predicted, as is demonstrated in the 1:1 comparisons in Fig. 2c.

Soil nitrate was under predicted by 126 kg N ha^{-1} in HN-NT and over predicted by 32 kg N ha^{-1} in HN-CT, with RMSE values of 315 and 50 kg N ha^{-1}, respectively (Table 3). Soil nitrate was under

Table 3
Observed and RZ-Shaw simulated soil nitrate-N content and change (Δ) in soil nitrate (kg ha^{-1}) in the 180 cm soil profile for high N (HN) and low N input (LN) of no-till and conventional till treatments from 2003 to 2006, with statistics (MD, mean difference; RMSE, root mean square error; r^2, coefficient of determination; and Nash-Sutcliffe model efficiency NMSE) between observed and simulated data.

| Tillage	N Rate	Soil NO$_3$-N kg ha^{-1}						soil Δ NO$_3$-N kg ha^{-1}	
		Obs	RZ	MD	RMSE	r^2	NSME	Obs	RZ
NT	HN	350	273	−126	147.8	0.45	0.27	399	275
	LN	61	43	−16.7	18.9	0.37	0.36	31	−10
CT	HN	208	235	32	65	0.52	0.29	205	221
	LN	31	68	37	39	0.11	−15.9	−15	−53

predicted in the LN-NT, with MD and RMSE values of 16.7 and 44 kg N ha^{-1}, respectively. Soil nitrate was over predicted in the LN-CT treatment, with an MD of 37 kg N ha^{-1} (Table 3). RZ-SHAW model accurately simulated net change (Δ) in soil NO_3-N over the measurement period (2003–2006) by: (1) predicting a larger increase in soil NO_3 for HN-NT compared to HN-CT; (2) little change for the LN-NT and; (3) a net a loss in the LN-CT treatment (Table 3). No-till systems may be more efficient at conserving soil N due to a larger SOC pool compared to a conventionally tilled system (Follett and Schimel, 1989). Lower soil nitrate levels measured in CT soils were partly a result of higher plant N uptake and higher rates of N_2O loss (Mutegi et al., 2010). Soil nitrate levels and crop N uptake were over predicted, but N_2O emissions were under predicted in both CT treatments (see N_2O discussion in Section 3.3), indicating that the soil N uptake routine may need further improvement (Fang et al., unpublished).

3.3. N_2O Emissions

Observed and simulated daily N_2O flux (g N ha day^{-1}) are presented in Fig. 3 during 2003–2006 for each tillage treatment. High precipitation led to rapid and sporadic N_2O losses immediately following N application in 2003 (Liu et al., 2005), leading to the highest emissions and demonstrating the influence of climate

on N_2O emissions across years (Lesschen et al., 2011). The 2003 measurement period is also a good example of the requirement to simulate complex environmental interactions regulating microbial nitrification and denitrification (Bessou et al., 2010; Fang et al., 2015). Two N_2O peaks were measured in 2003 from HN tillage treatments following the urea fertilizer applications (Fig. 3). There are often two N_2O peaks after fertilizer application, the first being from nitrification during the transformation of urea to NH_4-N; then the product of nitrification, NO_3-N, provides the necessary substrate for N_2O emissions from denitrification (Skiba and Smith, 2000). RZ-SHAW predicted two N_2O peaks from HN fertilized treatments, however while the model correctly predicted an initial high surge of N_2O, the duration was under estimated, resulting in under predicted cumulative emissions during 2003 (Fig. 3). Models have typically been unable to predict high N_2O fluxes from intensively managed agricultural systems of temperate region (Beheydt et al., 2007; Del Grosso et al., 2008). For this analysis, simulated N_2O emissions were likely improved by the more sophisticated sub-hourly accounting of daily soil water content in the RZ-SHAW model compared to the tipping bucket method simulated within the DAYCENT model as used by Del Grosso et al. (2008).

Lower N_2O emissions were measured in both tillage systems following fertilizer application in 2004 compared to those
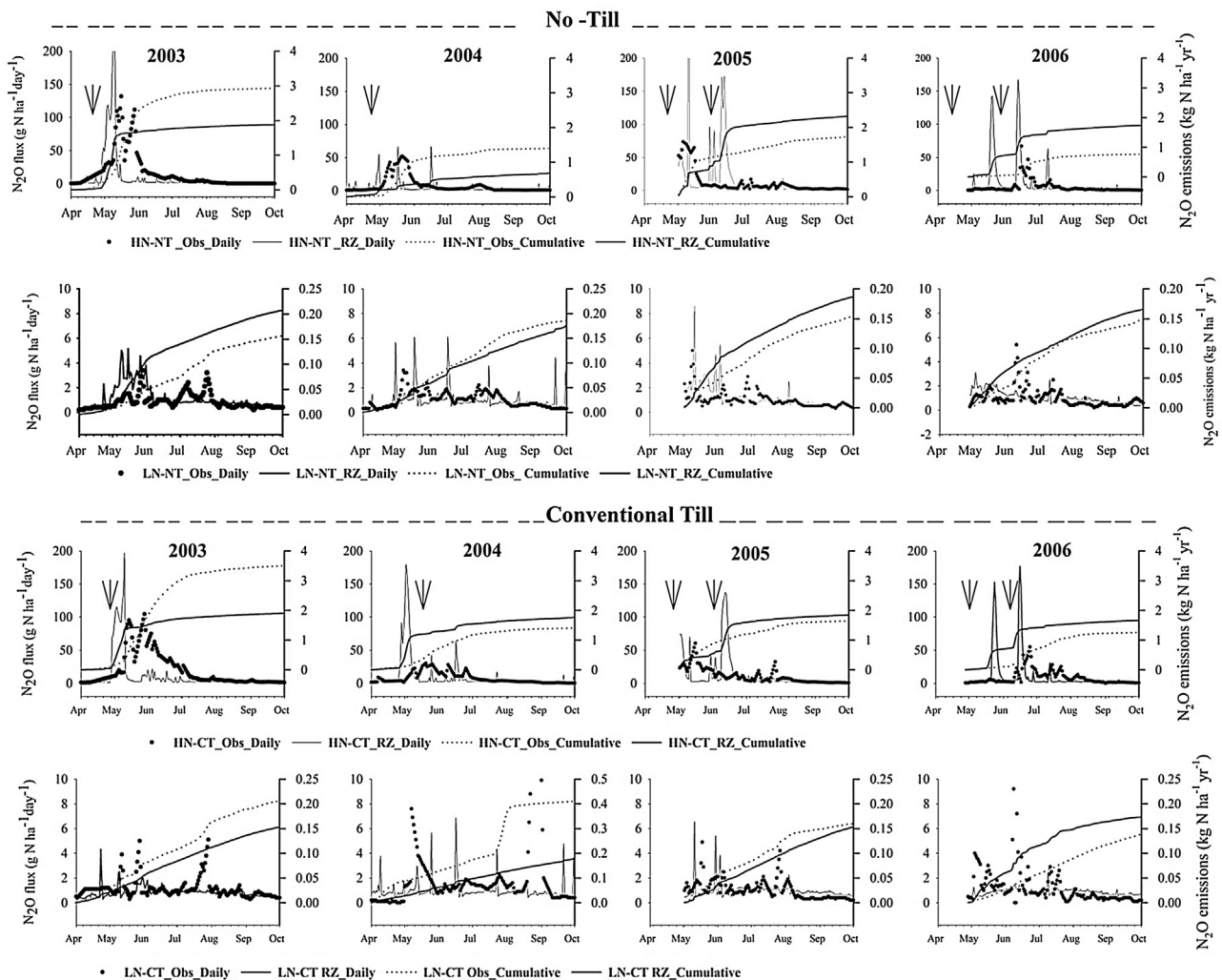
Fig. 3. Observed (closed circles) and RZ-SHAW (RZ) simulated (solid line) daily nitrous oxide flux (g N_2O-N ha^{-1} day^{-1}) from high no-till (NT) and conventional-till (CT) high N (HN) and low N input (LN) treatments in irrigated corn from 2003 to 2006. Second Y axis is observed (dotted line) and RZ-SHAW (RZ) simulated (solid) cumulative N_2O emissions (kg N_2O-N ha^{-1} yr^{-1}). Arrows indicate fertilizer applications to HN tillage treatments.

measured in 2003 (Fig. 3). There was no significant tillage effect over the 2003 and 2004 study period (Liu et al., 2005). Instead of one low N_2O peak that lasted for several weeks, as observed in the HN-NT treatment during 2004, RZ-SHAW simulated three small N_2O peaks, resulting in an under prediction of annual emissions by 0.71 kg N_2O-N ha^{-1} (Fig. 3). Conversely, peak fluxes were slightly over-predicted in the HN-CT treatment and slightly under predicted in the HN-NT (Fig. 3), causing simulated emissions in the HN-CT to be twice as high as the HN-NT treatments during 2004. High N_2O fluxes were measured in the LN-CT treatment during the late season of 2004, increasing annual emission to 0.5 kg N_2O-N ha^{-1} (Fig. 3). The failure to simulate these late season fluxes in LN-CT treatment caused emissions to be under predicted by approximately 50% in 2004 (Fig. 3).

Halvorson et al. (2008) evaluated N_2O emissions from the CT and NT tillage treatments during 2005 and 2006 using a spilt application of conventional (UAN in 2005 and urea in 2006) and an enhanced efficiency (polymer-coated urea (PCU)) fertilizer for high N rate treatments. Observed and simulated emissions ranged between 0.2 and 0.15 kg N_2O ha^{-1} yr^{-1} in the LN tillage treatments during 2005 and 2006 (Fig. 3). In the field experiment there was a significant N rate by year interaction for the HN treatments caused by significantly higher emissions in 2005 than in 2006. Field measurements showed similar emissions between HN-CT and HN-NT during 2005, totaling 1.6 and 1.75 kg N_2O-N ha^{-1}, but the HN-CT treatment had higher emissions than HN-NT treatment during 2006, that totaled 1.25 and 0.75 kg N_2O-N ha^{-1}, respectively (Halvorson et al., 2008). In the field, the PCU fertilizer applications did not result in rapid N_2O fluxes from either HN treatment during 2005 or 2006 (Fig. 3). The poly-coated technology is designed to release more N as soil temperature increases, slowing the release of urea and inhibiting N_2O fluxes by limiting N availability to microbial processes (Halvorson et al., 2008; Olson-Rutz et al., 2011; Halvorson et al., 2014). The RZWQM model however does not simulate slow N release mechanisms from enhanced efficiency fertilizers such as those formulated in the PCU fertilizer; therefore the low fluxes from the HN-NT treatment were over predicted especially after the first fertilization 2006 simulation period, where predicted emissions were nearly twice as high as the observed.

Cumulative emissions during the four years, 2003–2006, fell within the mean standard errors of the three field replicates over the four year measurement period for all treatments (Table 4). Field measurements indicated HN-NT treatments had slightly lower N_2O emissions (12%) than the HN-CT treatment. RZ-SHAW simulated N_2O emissions were slightly under predicted by 0.10 (1.5%) and 0.56 (7.1%) kg N ha^{-1} for HN-NT and HN-CT treatments, respectively, with corresponding NSME values of 0.58 and 0.69. Overall, N_2O fluxes in response to tillage were satisfactorily simulated, especially in that RZ-SHAW predicted slightly lower emissions (10%) from the HN-NT treatment compared to HN-CT treatment (Table 4). However while simulated N_2O emissions were similar to observed in HN-NT treatment, emissions were under predicted during 2003 and 2004 and over predicted during 2005 and 2006 (see HN-NT Fig. 3). Simulated N_2O emissions were over predicted in the LN-NT treatment by 0.11 (16%) kg N ha^{-1}, with a corresponding NSME value of 0.87. RZ-SHAW under predicted emissions by 0.29 (29%) kg N ha^{-1} in the LN-CT treatment (Table 4), resulting in a slightly lower NSME value of 0.5. However, this was mostly an effect of under predicted emissions during the late 2004 growing season. By excluding the late 2004 measurement period, simulated emissions were within 1.3% of the observed, and increased the NSME value to 0.97 for the LN-CT treatment.

In order to demonstrate the capability of the RZ-SHAW model to predict seasonal N_2O emission trends throughout the growing season, seasonal N_2O emissions (early (April–June), mid (July–August), and late (September–October)) were averaged for each treatment (Fig. 4). Differences between measured and simulated early-season N_2O emissions for HN-NT treatments are notable (Fig. 4a), but importantly high standard errors are often associated with high N_2O fluxes from field measurements (Halvorson et al., 2008). There were strong positive correlations (R^2) between measured and simulated for seasonal N_2O emissions in the HN tillage treatments (~ 0.6), and slightly lower correlations for LN treatments (~ 0.3), see Fig. 4. Theoretically process based models should be able to predict seasonal variability of N_2O emissions (Cai et al., 2003). Yet previous efforts to simulate emissions from these field plots using DAYCENT resulted in a 50% over prediction of N_2O emissions caused by high simulated mineralization rates during the latter part of the growing season (Del Grosso et al., 2008).

3.4. Emission factors and GHG intensity

Observed and simulated emission factors (EF) [=(N_2O emission at N rate – N_2O emission at zero N rate)/N rate) were 0.66 and 0.65% for HN-NT and 0.75 and 0.70% for HN-CT treatments, respectively. The IPCC Tier I methodology uses an EF of 1% for applied fertilizer (IPCC, 2006). Because the Tier I approach does not account for spatial and temporal variation of climate and soil (Lesschen et al., 2011), N_2O emissions would be over predicted by 30 and 20% using the Tier I approach for HN-NT and HN-CT, respectively. Contrary to the Tier I approach, we show that using a validated ecosystem model in conjunction with measured data improves the reliability of simulated N_2O emission, as suggested by IPCC Tier III methodology (IPCC, 2006; Metivier et al., 2009).

Greenhouse gas (GHG) intensity provides an estimate of emissions per unit of yield (Mg ha^{-1}), and are converted to kg of carbon dioxide equivalents (CO_2e) based on the 100 year global warming potential of 298 for N_2O (Eggleston et al., 2006). Measured GHG intensities were 54.8 and 57.8 kg CO_2e Mg grain^{-1}

Table 4

Observed and RZ-SHAW simulated N_2O emissions (kg N ha^{-1}) during the four year study period (2003–2006) from no-till (NT) and conventional-till (CT) high N (HN) and low N input (LN) treatments. Comparisons between observed and RZ-SHAW simulated N_2O emissions using Nash-Sutcliffe model efficiency (NMSE); r^2, coefficient of determination; (MD, mean difference; RMSE, root mean square error. Greenhouse gas (GHG) intensity is calculated from observed and simulated N_2O emissions (converted into carbon dioxide equivalent (CO_2e) by using Global warming potential of 298) and divided by the respective grain yields (Mg) over the 2003–2006 study period.

Tillage	N Rate	N_2O kg N ha^{-1} yr^{-1}							GHG intensity CO_2e Mg grain yield^{-1}	
		Obs	ste*	RZ-SHAW	MD	RMSE	r^2	NMSE	Obs	RZ-SHAW
NT	HN	6.88	5.67	6.78	0.05	1.85	0.77	0.58	54.8	54.5
	LN	0.62	0.70	0.79	−0.05	0.20	0.52	0.87	11.9	10.7
CT	HN	7.85	4.91	7.29	0.28	1.98	0.50	0.69	57.8	53.0
	LN	0.98	0.80	0.69	0.15	0.31	0.50	0.51	13.1	8.9

Mean standard error (ste)* of three replications from daily N_2O flux during 2003–2006.

No-Till
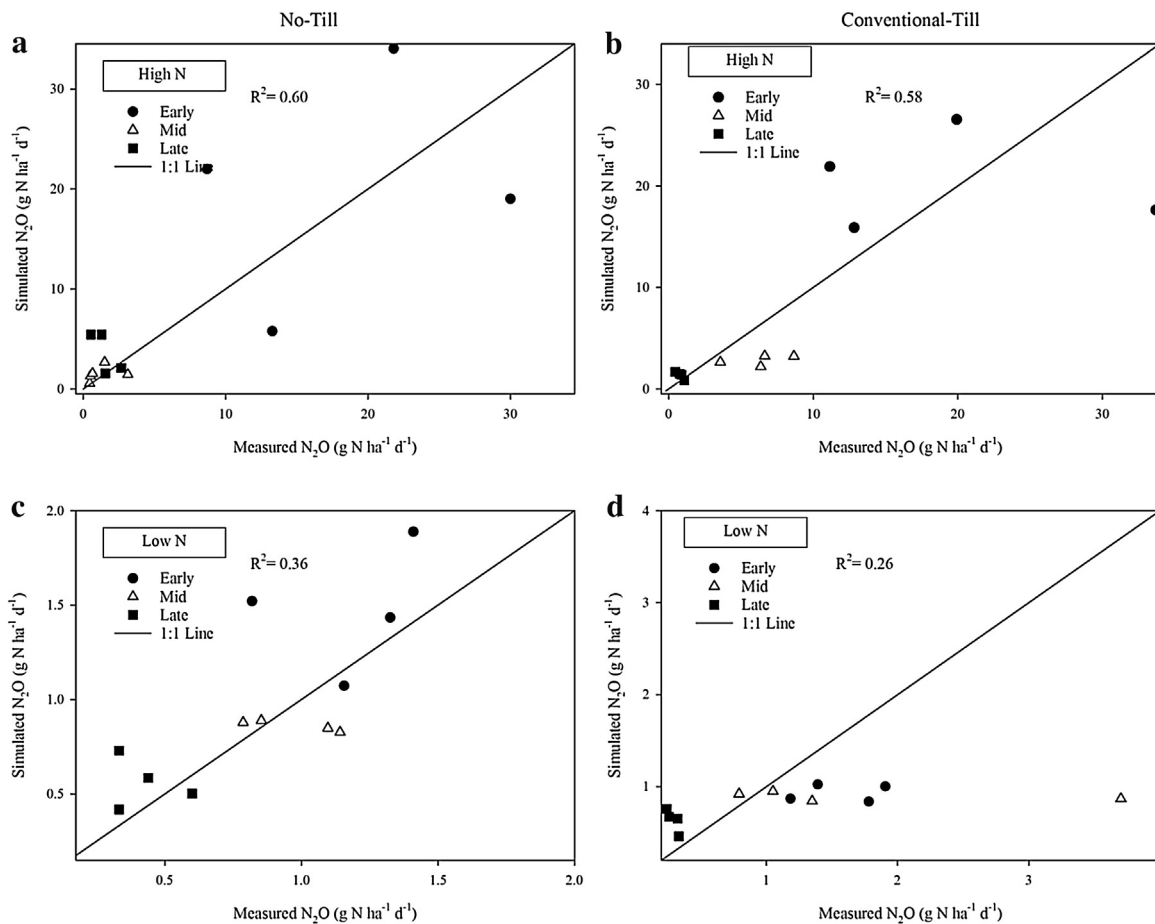
Conventional-Till

Fig. 4. Observed and simulated seasonal N_2O emissions ($g\,N\,ha^{-1}\,day^{-1}$) from no-till and conventional-till high N (HN) (a and b) and low input (LN) treatments (c and d) during the early (April–June), mid (July–August), and late (September–October) growing season of 2003–2006.

for HN-NT and HN-CT treatments, and 11.9 and 13.1 kg CO_2e Mg grain^{-1} for LN-NT and LN-CT treatments, respectively (Table 4). Based on simulated crop yield and N_2O emissions, there was less than a 1% difference between observed and simulated GHG intensity for HN-NT, and less than 10% difference for the LN-NT and HN-CT (Table 4). There was a larger disagreement between observed and simulated GHG intensity for LN-CT which under predicted GHG intensity by 32%, caused by an under prediction of N_2O emissions and an over prediction of crop yield. Our analyses however demonstrate the potential of using RZ-SHAW to investigate the multifaceted challenges between field management and environmental impacts.

3.5. Mineralization and denitrification

The soil contained 2.1% soil organic matter (SOM) (Halvorson et al., 2006). For every 1% of SOM approximately 35 kg N ha^{-1} is mineralized per growing season (Vigil et al., 2002). Simulated

mineralization from 2003 to 2006 was approximately 60 kg N ha^{-1} yr^{-1} for the LN tillage treatments, and is therefore within the range of the expected value (Table 5). To verify the higher mineralization rates from HN treatments, a partial soil N balance (Karlen et al., 1998) can be calculated by assuming the conservation of mass:

$$\sum Ninput - \sum Noutput - \Delta soilN = residual soilN \qquad (15)$$

Higher biomass N content in the HN treatments increases availability of mineralizable N compared to LN treatments; here we estimate that about 45 kg N ha^{-1} yr^{-1} more is cycled in the HN treatments. Importantly, RZ-SHAW predicted higher mineralization rates (12 kg N ha^{-1}) in the HN-CT treatments than in the HN-NT treatments (Table 5). That is, the incorporation of surface residue increased organic inputs by 50% and increased mineralization rates by over 10% in HN-CT compared to HN-NT (Table 5). These suggested differences in N cycling were an important factor affecting N_2O emissions between tillage systems. Limited mixing of surface residue and soil in NT systems may slow decomposition

Table 5
Simulated partial N budget for no-till (NT) and conventional till (CT) high N (HN) and low N (LN) rate treatments (mean values from 2003 to 2006).

Tillage	N Rate	N_2O from Nitrification kg N ha^{-1}	Denitrification kg N ha^{-1}	Mineralization kg N ha^{-1}	N_xO N kg N ha^{-1}
NT	HN	1.77	21.6	102.3	1.40
	LN	0.29	0.95	63.4	0.21
CT	HN	1.82	19.5	114.9	2.0
	LN	0.28	0.86	59.8	0.29

rates, causing differences in N cycling between tillage systems and influencing soil N_2O emissions (Follett and Schimel, 1989; Quemada and Cabrera, 1997). Crop simulation models that can account for differences in N cycling through residue management may help improve estimates of N_2O emissions (Delgado et al., 2010).

Biological nitrification was the main parameter adjusted in the new RZWQM2-GHG simulation component (Fang et al., 2015), as this was the primary pathway for N_2O emission in this semi-arid system (Mosier et al., 1996). RZ-SHAW predicted that 90–95% of N_2O was emitted through microbial nitrification, and that HN-NT had nearly 10% higher denitrification rates (Table 5). At these field plots, Liu et al. (2005) measured lower nitric oxide (NO) emissions from NT fertilized plots, caused by wetter and less aerated soil conditions which increased microbial denitrification. Gas diffusion is slowed in soils with higher soil water content or greater microporosity, enabling NO to be further reduced to N_2O (Conrad, 1996; McTaggart et al., 2002). Also, RZ-SHAW predicted 30% higher aerobic microbial activity in CT compared to NT treatments (data not shown). Soil aggregates are reconsolidated within the RZWQM2 model due to fewer soil disturbances under NT management. Soil disturbance from tillage management can alter the functional groups of microbial communities causing differences in denitrification rates (Cavigelli and Robertson, 2001). Ecosystem crop models enhance field research by offering a comprehensive evaluation of multiple biological processes (Ahuja and Hatfield, 2007; Zhang et al., 2013), and can lead to new investigative research (Oreskes et al., 1994). Model results presented here have shown that tillage management caused differences in N cycling and microbial communities between NT and CT systems.

4. Conclusion

This study is the first evaluation of the newly added GHG component to RZ-SHAW under different tillage systems. RZ-SHAW closely predicted crop yield and biomass over the four year study period (2003–2006) for all tillage treatments. By accounting for residue insulation effects on the soil surface, lower early season surface soil temperatures were correctly predicted in NT compared to CT treatments. However, there were several discrepancies between observed and simulated daily N_2O fluxes. For example, the initial surge of simulated N_2O flux was too high and the duration was too short during the 2003 simulation period, resulting in an under prediction of N_2O for HN treatments. The model failed to simulate the slightly higher annual emissions from LN-CT compared to LN-NT, though this was primarily caused by high N_2O measured during the late 2004 growing season. Emissions from HN-NT were over predicted in 2005 and 2006 when enhanced efficiency fertilizers were applied as the respective second and first treatment applications. Nevertheless, the strong correlations between measured and simulated N_2O emissions indicate the model made accurate predictions on a seasonal basis. Observed and simulated cumulative N_2O emissions from 2003 to 2006 were also in close agreement, with 12 and 10% lower emissions from HN-NT compared to HN-CT, respectively. Model output showed differences in N cycling between tillage treatments, indicating lower organic residue inputs and higher denitrification rates lowered simulated N_2O emissions in HN-NT. Overall, RZ-SHAW simulated N_2O emissions were reasonable between the different N and tillage treatments of this irrigated corn system, and may be applicable to other agricultural practices within the region. Deserving further attention is the slowed diffusion rates of urea hydrolysis when using enhanced efficiency fertilizers within RZ-SHAW model, as this would add model support to N_2O mitigation strategies.

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