Calibration and validation of the DNDC model to estimate nitrous oxide emissions and crop productivity for a summer maize-winter wheat double cropping system in Hebei, China

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Key words: Calibration; Validation; Nitrous oxide; DNDC model; Crop productivity; Summer maize-winter wheat double cropping system.

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Abstract

The main aim of this paper was to calibrate and evaluate the DeNitrification-DeComposition (DNDC) model for estimating N_2O emissions and crop productivity for a summer maize-winter wheat double cropping system with different N fertilizer rates in Hebei, China. The model's performance was assessed before and after calibration and model sensitivity was investigated. The calibrated and validated DNDC performed effectively in estimating cumulative N_2O emissions (coefficient of determination (1:1 relationship; r^2) = 0.91; relative deviation (RD) = -13 to 16%) and grain yields for both crops (r^2 = 0.91; RD = -21 to 7%) from all fertilized treatments, but poorly estimated daily N_2O patterns. Observed and simulated results showed that optimal N fertilizer treatment decreased cumulative N_2O flux, compared to conventional N fertilizer, without a significant impact on grain yields of the summer maize-winter wheat double cropping system. The high sensitivity of the DNDC model to rainfall, soil organic carbon and temperature resulted in significant overestimation of N_2O peaks during the warm wet season. The model also satisfactorily estimated daily patterns/ average soil temperature (^{o} C; 0-5 cm depth) (r^2 = 0.88 to 0.89; root mean square error (RMSE) = 4^o C; normalized RMSE (nRMSE) = 25% and index of agreement (d) = 0.89-0.97) but under-predicted water filled pore space (WFPS; %; 0-20 cm depth) (r^2 = 0.3 to 0.4) and soil ammonium and nitrate (exchangeable NH_4^+ & NO_3^-; kg N ha^{-1}; r^2 = 0.97). With reference to the control treatment (no N fertilizer), DNDC was weak in simulating both N_2O emissions and crop productivity. To be further improved for use under pedo-climatic conditions of the summer maize-winter wheat double cropping system we suggest future studies to identify and resolve the existing problems with the DNDC, especially with the control treatment.

Capsule

The calibrated DNDC model effectively estimated cumulative N_2O emissions, grain yields and soil temperature but underestimated WFPS and soil N, in a winter wheat-summer maize double cropping system.

Key words: Calibration; Validation; Nitrous oxide; DNDC model; Crop productivity; Summer maize-winter wheat double cropping system.

1 Introduction

Quantification of greenhouse gas (GHG; CO_2, CH_4 and N_2O) emissions from agricultural soils is essential for developing mitigation options and policies. However, this requires establishing and maintaining field flux measurement sites which are time consuming and expensive. Well-calibrated simulation models for GHG emissions offer an opportunity to complement physical experiments by employing computers to calculate the likely outcomes of different physical phenomenon (Giltrap et al., 2010). Nitrification and denitrification are the main processes responsible for N_2O production in soils and their contribution depends on the environmental conditions (Mathieu et al., 2006). Simulation models have the ability to simulate relationships between soil physical, chemical and microbial processes that underpin nitrification, denitrification and decomposition. They also allow complex interactions and real-world problems to be examined in a time effective way, by applying mathematical knowledge and computational power. Moreover, simulation models can support decision makers by facilitating the understanding of a system and allow potential mitigation strategies of GHG emissions, and a range of climate change-land use change scenarios to be examined (Giltrap et al., 2010).

Simulation models are very diverse and range from simple empirical relationships based on statistical analyses to complex mechanistic models that consider numerous soil-climate-crop parameters controlling and influencing GHG production and emissions from soils (Roelandt et al., 2005; Jinguo et al., 2006). The exact estimation of the trace GHG, nitrous oxide (N_2O), emissions from soil is difficult and represents a challenge for most of the models which perform over a wide range of conditions. However, soil parameters and almost all processes responsible for production, consumption and transport of this gas can be simulated (Willams et al., 1992). One of the process models used to estimate N_2O emissions is the DeNitrification-DeComposition (DNDC) model. The DNDC model is a biogeochemical model used to estimate soil GHG emissions and crop production. Although it was initially developed for conditions in the USA (Li et al., 1992, 2000), it has been used for simulating N_2O emissions worldwide e.g. in Canada (Smith et al., 2010), Europe (Kesik et al., 2006; Abdalla et al., 2009) and extensively in China (Deng et al., 2011; Hu et al., 2012).

China is facing the dual challenge of increasing crop production for its growing population while at the same time reducing its GHG emissions. Therefore, a plan for improving agricultural management practices to promote grain yields and minimize GHG emissions is needed (Chen et al., 2014). Two of the primary cereal crops in China are maize and wheat which are grown on an area of about 42 and 24 million ha (FAO, 2017), respectively. Maize is also an important forage crop, where about 68% of its production in China is used for animal feed (Ely et al., 2016). Summer maize-winter wheat double cropping system is a common cropping system in the North China plain. Previous studies found that crop rotation/ double cropping system positively increased crop yields compared to monoculture management (Laik et al., 2014). However, both the maize and wheat crops require a large amount of N fertilizer for optimum growth and production. In addition, farmers commonly overuse N fertilizer or apply a low efficiency types (Li et al., 2012). They usually add 30-60% more N fertilizers than the level required for optimum crop yields (Norse, 2011). However, overuse of N fertilizer has recently started to decline in some areas and the government set a policy of zero growth in N fertilizer and pesticide use by 2020 (Powlson et al., 2018).

Nitrous oxide is a potent GHG. The emission of this gas from agriculture is produced through biological processes in soils and the degree of variation (spatial and temporal) in the emissions depends on soil type, land use and climatic factors (e.g. rainfall, temperature) (Conrad, 1996). The inorganic N pool provides electrons for producing energy during nitrification whilst, organic C provides electrons to reduce combined N during denitrification (Addiscott et al., 1983; Khalil et al., 2002). Unfavourable management practices result in high N_2O emissions which are mainly controlled by available N and C in soils (Galloway 1998; Ding et al. 2007). Management can also influence soil fertility, indirectly, through management-induced changes in plant composition (Collins et al., 1998; Patra et al., 2006) and thereby, increase gas fluxes.

Modelling of a double / multiple cropping system is still a challenge because of the hysteresis influence on soil properties such as soil moisture, nutrients and soil organic C (SOC). Over the past 25 years many developments have been made to the DNDC model to meet the needs of users. These include, among others, modularization of the code structure (Haas et al. 2013), and development of an integral optimisation function for crop and other input parameters (Lamers et al., 2007; Van Oijen et al., 2011). However, to the best of our knowledge, the model has not previously been calibrated for a summer maize-winter wheat double cropping system in China. The main aim of this paper was to calibrate and evaluate the DNDC model for estimating N_2O emissions and crop productivity for a summer maize- winter wheat double cropping system with different N fertilizer rates in Hebei province, the North China plain. Additionally, the ability of the model to estimate soil variables of temperature, water filled pore space (WFPS) and soil N (exchangeable NH_4^+ and NO_3^-) was assessed. Results are discussed in terms of highlighting the strengths, weaknesses and potential future improvements to the DNDC model for simulating the double cropping system in China.

2 Materials and methods

2.1 Experimental site

This study used the data published in Song et al. (2018) to calibrate and validate the DNDC model. An experiment was set up in Quzhou county, Hebei province, to investigate the impacts of N management on N_2O emissions. As detailed in Table S1, five N treatments with four replicates in a fully randomized block design were investigated. These treatments were: control (no N fertilizer); conventional N (the amount of N fertilizer used in current practice; see Table S1); the other three treatments were designed with optimized fertilizer N rates, namely: optimal N; 0.7*optimal N and 1.3*optimal N fertilizer (*= means multiplication). Optimal N fertilizer was calculated by the in-season root zone N management strategy to mitigate GHG emissions (Cui et al., 2013). Here, soil N ($NH^+{}_4{}^-N$ and $NO^-{}_3$-N) in the root zone was subtracted from the target N values for the growing period. Further details about the site, crop, soil parameters and management are shown in Song et al. (2018).

2.2 Field measurements

2.2.1 Temperature and precipitation

Mean daily air temperature and precipitation were collected from the weather station at the study site (Fig. S1) as described by Song et al. (2018).

2.2.2 Fluxes of N_2O

Measurements of N_2O fluxes were carried out throughout the experimental period from June 2012 to June 2014, using the closed static chamber method. Gas samples were collected on a daily basis for 10 days after application of N fertilizer and 3 days after irrigation or rainfall (>20 mm). However, for the remaining periods, the gas was sampled every 4 days, except in winter when the gas was sampled weekly. More details about N_2O measurements can be found in Song et al. (2018).

2.2.3 Calculation of N_2O flux

The daily N_2O flux was calculated as shown in Song et al. (2018).

2.2.4 WFPS (%) and soil N (exchangeable NH_4^+ and NO_3^-)

Soil samples for measurements of WFPS and mineral N (exchangeable NH_4^+ and NO_3^-) were collected and calculated as described in Song et al. (2018).

2.3 Model description

DNDC v. 9.5 is a biogeochemistry model which describes the soil C and N cycles and GHG fluxes from agricultural systems (Gilhespy, 2014). The DNDC model accommodates six sub-models (Li et al., 1992, 2000).

2.4 Model's calibration and sensitivity analysis

This study represents a further step of our previous studies to investigate the suitability of the DNDC model for estimating N_2O, crop yield and soil properties for China's cropland (Song et al., 2018; Yue et al., 2018). The DNDC model was calibrated to produce measured crop yields / cumulative N_2O emissions for the site using the measured data from the 0.7 * optimal N treatment. Data from the control plot were not used for calibration because there were many days in the control data in which the measured N_2O flux was negative and negative fluxes are not simulated by DNDC.

Model calibration for crop yields and cumulative N_2O emissions was done by optimizing a combination of different crop growth parameters (maximum biomass production, biomass fraction, biomass C/N ratio, thermal degree days, water demand and optimum temperature) and adjusting SOC inputs, respectively. Different crop parameters/ SOC input default values were tested until the model matched the measured grain yield/ cumulative N_2O flux values (Table 1). The grain yield was measured in t ha^{-1}. The calibrated model was then used to run the other 4 treatments (control, conventional N, optimal N and 1.3 * optimal N).

The sensitivity of the DNDC model and the attribution of N_2O and summer maize/ winter wheat grain yields to different input parameters were investigated to quantify the effects of these parameters on the N_2O emissions and grain yields (Smith and Smith, 2007; Abdalla et al., 2009a). We change only one parameter at a time and kept the other ones constant. Simulations were run to assess how N_2O and grain yields were influenced by different climate parameters: average daily temperature (increased/ decreased by a range from1 to 3° C with an increment of 1° C) and average daily rainfall (increased/decreased by a range from -30% to +30% with an increment of 10%). The model was also run to see how N_2O and grain yields were affected by changes in SOC and for the amount of N fertilization rate and water irrigation. SOC, N fertilizer and irrigation were changed by -30% to +30% with an increment of 10%.

2.5 Model run, validation and statistical evaluation

To run the DNDC model, climate, soil and management data including N fertilizer, irrigation and tillage were input into the model. These are summarized in Tables 1, 2 and 3. The model testing was carried out by comparing (1) simulated and observed daily/ cumulative N_2O fluxes (2) simulated and observed crop grain yields and (3) simulated and observed soil N (exchangeable NH_4^+ and NO_3^-) (4) simulated and observed soil moisture in terms of WFPS (5) simulated and observed soil temperature. The model was validated by comparing observed and simulated values.

The model accuracies were evaluated by calculating root mean square error (RMSE; equation 1), normalized RMSE (nRMSE; equation 2), index of agreement (d; equation 3) Yang et al. 2014) and modelling efficiency (EF; equation 4) (Nash and Sutcliffe, 1970). Using these indices help us to quantify the overall model performance. The RMSE have the same unit of simulated and observed values, whilst nRMSE is a relative measure. The d ($0 \leq d \leq 1$) gives the degree of deviation towards zero. EF ($-\infty$ to 1) compares the ability of the model to reproduce the daily data variability based on the arithmetic mean of the measurements. Negative EF value shows a poor performance, a value of 0 indicates that the model does not perform better than using the mean of the observations, and values close to 1 indicate a ‘near-perfect’ fit.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(S_i - M_i)^2}{n}} \qquad (1)$$

$$nRMSE = \frac{RMSE}{\bar{M}} \times 100 \qquad (2)$$

$$d = 1 - \frac{\sum_{i=1}^{n}(S_i - M_i)^2}{\sum_{i=1}^{n}\left(|S_i - \bar{M}| + |M_i - \bar{M}|\right)^2} \qquad (3)$$

$$EF = 1 - \frac{\sum_{i=1}^{n}(S_i - M_i)^2}{\sum_{i=1}^{n}\left(M_i - \bar{M}\right)^2} \qquad (4)$$

The relative deviation (RD; %) of the observed values from modelled ones was also calculated as follow:

RD = (Mi-Si)/Mi (5)

Where S_i is the simulated value, M_i is the measured value, n is the number of measured values, and $\bar{M}$ is the average of the measured values. Cumulative flux for models results were determined by the summation of modelled daily emissions over the experimental period (Cai et al., 2003). Additionally, coefficient of determination (r^2), which is the correlation between simulated and observed values was used to assess whether simulated values follow the same pattern as observed values.

3 Results

3.1 Model's calibration

The adopted combination of crop parameters used for DNDC- calibration was shown in Table 2. The calibrated DNDC model successfully produced the exact measured crop yields (t ha^{-1}) of the 0.7*optimal N treatment for each crop/ season. Likewise, the input amount of SOC at 0-10 cm in the model was adjusted to 0.021 kg C kg^{-1} soil (i.e. SOC value resulted from the model calibration) and the model also gave the measured cumulative N_2O flux for the 0.7* optimal N treatment of 5.4 kg N_2O-N ha^{-1}.

3.2 Model sensitivity analysis

The sensitivity of the DNDC-model to the essential input parameters (i.e. rainfall, air temperature, SOC, N fertilizer rate and water irrigation) for simulating cumulative N_2O flux for the summer maize-winter wheat double cropping system was tested. The model was found to be sensitive to changes in all of these parameters but to different extents (Fig. 1). The greater response was to rainfall, where changing daily rainfall by a range from -30% to 30% changed the cumulative N_2O emissions by a range from -50% to 42%. Changing SOC by a range from about -30% to 30% changed cumulative N_2O emissions by a range from -36% to 39%. The DNDC was also sensitive to changes in daily air temperature (^oC) and N fertilizer application rate. Changing daily air temperature and N fertilizer by a range from -3 ^oC to 3^oC and from -30% to 30% changed cumulative N_2O by ranges of -16% to 12% and -22% to 12%, respectively. However, the model was less sensitive to irrigation where changing irrigation by a range from -30% to 30% changed cumulative N_2O emissions by a range from -1% to 2%, respectively. Here, increasing water irrigation had slight negative influence on the cumulative N_2O emissions from soil.

3.3 Evaluation of the DNDC model

3.3.1 Nitrous oxide emissions

The DNDC model was able to predict timing of the daily observed N_2O flux peaks from all N treatments during the two crop rotations, with few exceptions, but significantly overestimated their magnitude (Fig. 2). These peaks appeared for all treatments including the controls on occasions where combinations of higher daily rainfall (mm) and air temperature (^oC) were observed. For the control treatment, observed and simulated N_2O flux peaks corresponded to higher daily rainfall and air temperature. However, the height of these peaks increased further relative to the amount of the N fertilizer added in each N treatment plot. The highest observed and simulated peaks were 6, 819, 149, 246 g N_2O-N ha^{-1} d^{-1} and 267, 831, 670 and 714 g N_2O-N ha^{-1} d^{-1} for the control, conventional N, optimal N and 1.3 *optimal N, respectively. For all treatments, RMSE ranged from 0.55 to 2.59 g N_2O-N ha^{-1} d^{-1}; nRMSE from 4 to 20%, d from 0.10 to 0.50 and EF was <0 (Table 2). Both the observed and simulated cumulative N_2O flux showed lower emissions from the optimal N fertilizer treatment compared to the conventional and 1.3*optimal N fertilizer treatments (Table 2). The model performed better, for both N fertilized and control treatments, after calibration compared to before calibration. Here, RD ranged from -13 to 16% compared to -46 to -54% for the N fertilized treatments, respectively (Table 2). However the model, generally, simulated daily/ cumulative N_2O flux for the control in both cases, poorly. The DNDC overestimated the flux for the control treatment by 68%

before model calibration and by 42% after calibration. Overall, the model simulated cumulative annual N_2O emissions from the maize-wheat double cropping system with an r^2 of 0.91 (1:1 relationship; Fig. S2).

3.3.2 Crop yields

With the exception of the control treatment, the DNDC model estimated observed grain yield from both crops (summer maize and winter wheat) and all N treatments, effectively. The model performed better after calibration, for both crops, compared to before calibration. For the N treatments, the RD for simulating summer maize and winter wheat after calibration ranged from -7 to 7% and from -21 to 6% compared to from 5 to 20% and from -42 to 59% before calibration, respectively. The RD for simulating summer maize and winter wheat for the control treatment after calibration ranged from -30% to -40% for the summer maize and from -50 to -60% for the winter wheat compared to -92% to -97% and -83% to -87% before calibration, respectively (Table 3). A 1:1 relationship showed that the DNDC simulated grain yield for summer maize with r^2 of 0.89 and r^2 of 0.92 for winter wheat. The overall r^2 of simulated and observed grain yields was 0.91 (Table 3; Fig. S3). On average, both the observed and simulated grain yields showed that the optimal N fertilizer treatment slightly reduced crop yields (by 1 to 2%) compared to the conventional and 1.3* optimal fertilizer treatments (Table 3).

3.3.3 Soil properties

The daily WFPS (%) during the experimental period was primarily driven by rainfall. Both the observed and simulated daily WFPS (%) corresponded well with increasing and decreasing of daily rainfall. The DNDC model simulated daily trends in WFPS (%; 0-20 cm depth) with some under-estimations of the observed values. 1:1 relationships showed that the model simulated fluctuations in WFPS% (0-20 cm depth) with r^2 ranging from 0.3 to 0.4 (Fig. S4). For all treatments the RD ranged from -62 to -76%. RMSE ranged from 12.9 to 42% and nRMSE from 24 to 74. The d values were ranged from 0.40 to 0.75 and EF from <0 to 0.10.

With exception of the control treatment, the DNDC model was able to estimate timing of soil N (exchangeable NH_4^+ and NO_3^-) peaks throughout the two rotations and all N treatments, reasonably well, although it poorly estimated their magnitude (Fig. 3). The model under-estimated the observed soil N peaks during periods of N application. The r^2 between the daily observed and simulated values ranged from 0.11 to 0.17 and was 0.97 for the cumulative soil N (1:1 relationship; Fig. S5). The RD ranged from -19 to -42% and RMSE ranged from 0.27 to 2.39 kg N ha^{-1}. The nRMSE values were small (2-4%); and d values were large (0.57-

0.75). The model significantly underestimated soil N for the control: (RD = -0.91; RMSE= 0.54 kg N ha^{-1}; nRMSE= 4% and d= 0.58 and EF ranged from <0 to 0.58 (Table 3; Fig. 3).

The DNDC model simulated daily trends in soil temperature (0-5 cm depth) throughout the two summer maize-winter wheat double cropping system, effectively with some slight over/ under-estimation of the observed values (Fig. 4). The variation in measured soil temperature, over the experimental period, was primarily derived by air temperature at the site. Both the observed and simulated soil temperatures at 0-5 cm depth were not significantly different between the different N treatments. The model simulated fluctuations in temperature (0-5 cm) during the wet season (i.e. summer months) better than during the dry season (i.e. winter months) (Figs. 1 and 5). A 1:1 relationship showed that the r^2 between the simulated and observed values ranged from 0.88 to 0.89 (Fig. S6) and overall RD was 20%. The EF ranged from 0.79 to 0.96 and RMSE was 4.1^{o} C and both nRMSE and d values were reasonable; 25% and 89-97, respectively (Table 3).

4 Discussion

4.1 Model calibration and sensitivity analysis

In this study, calibration and validation of the DNDC model using 0.7*optimal N treatment was required because of the differences in the crop types and environment (i.e. DNDC was originally developed for crop growth and environment in the USA). The calibration of DNDC, especially for crop growth, is critically important due to the greater impacts of cropping systems on soil N, C and water dynamics and thereby on the daily/ cumulative values of N_2O emissions and other biogeochemical processes (Zhang and Niu 2016). The use of the 0.7*optimal N treatment, for which there are independent data, for model calibration was essential. Many previous studies recommended calibration and validation of the DNDC model to improve the accuracy of the model key biogeochemical processes (e.g. Tonitto et al. 2007; Li et al. 2014). Our calibrated and validated model gave better estimation for cumulative N_2O flux and crop grain yields.

The model sensitivity analysis for simulating N_2O flux showed that the DNDC model is very sensitive to some climate, soil and management parameters including rainfall, temperature, N fertilizer and SOC but less sensitive to water irrigation rate as shown in Fig. 1. The DNDC was more sensitive to these parameters than in the study reported by Abdalla et al. (2009a). This may be due to differences in the DNDC versions applied, soil texture, management and environmental variables of the two sites. Rainfall increases both field measured/ simulated soil moisture and thereby stimulates soil denitrification by lowering oxygen dispersal into the soils (Abdalla et al. 2009b; Song et al. 2019). It also makes soil organic C and nitrate more prone to denitrification processes by increasing their solubility (Bowden and Bormann 1986). Therefore, rainfall events result in higher N_2O flux peaks/ cumulative flux as shown by Ludwig et al. (2011), Abdalla et al. (2012) and others. Water irrigation also stimulates N_2O emissions (Yan et al. 2015). However, increasing water irrigation rate can result in conditions of a complete denitrification in which N_2O is further reduced to N_2 (Conrad 1994) and consequently decrease N_2O emissions. This is why slightly negative effects on the N_2O flux were observed in this study. In a two year study Kuang et al. (2018) reported that flood irrigation decreased N_2O emissions, compared to drip irrigation, in one year and had no significant difference in the second year.

Similar DNDC sensitivity to the higher air temperature found in this study, was also reported by Abdalla et al. (2009a). This is interesting, and could result in significantly higher N_2O emissions in the future especially because North China (area of this study) is projected to change towards warmer and more humid conditions, and both rainfall and temperature will increase as reported by Chu et al. (2017). The DNDC was sensitive to both additional synthetic N fertilizer input and SOC. Changes in the amount of N fertilizer application rate has a direct and a strong impact on N_2O emissions by making N available for the processes of nitrification and denitrification in soils (Baggs and Blum, 2004). The N released to the atmosphere rely on the amount of N used up by the crop (Abdalla et al., 2010). However, the overuse of N fertilizer and application of a low use efficiency types in China (Li et al., 2012), if it continues, would worsen the situation further. We found that the optimal N fertilizer treatment decreased cumulative N_2O flux, compared to conventional and 1.3*optimal N fertilizer treatments, without having a significant impact on grain yields of either crop. Hu et al. (2012) reported that splitting the fertilizer into more applications reduced N_2O emissions from spring maize. Moreover, using the same data used in this study, Song et al. (2018) found that cumulative and yield-scaled N_2O emissions increased exponentially as N applications were raised above the optimum rate in maize (*Zea mays* L.) and have quadratic increases in winter wheat (*Triticum aestivum* L.).

4.2 Evaluation of the DNDC model for simulating crop rotation

4.2.1 Nitrous oxide emissions

In this study, although the DNDC correctly simulated the timing of most daily N_2O flux peaks from all N treatments, it significantly overestimated their magnitudes. These peaks appeared also in the control treatment and corresponded to combinations of higher daily rainfall and temperature (the model is very sensitive to both parameters). Similar peaks at higher daily rainfall events and temperature were simulated by Ludwig et al. (2011) and Abdalla et al. (2012). These factors stimulate N_2O fluxes as they provide more substrate and favourable conditions for both denitrification and nitrification in soils (Abdalla et al., 2014). Davidson et al. (1993) and Huang et al. (2014) reported that under dry climate and low soil moisture, nitrification was the main process behind N_2O production. The magnitude of the flux peaks increased relative to the amount of added N in each treatment with the largest peak appearing in the conventional N, and the lowest peak in the optimal N treatment. Li et al. (2012) reported that avoiding application of N fertilizers coincident with heavy rainfall events can reduce N_2O emissions from spring maize production in Northeast China. However, to reduce measured/ simulated N_2O emissions without significantly affecting crop yield, application of N fertilizer should be decided depending on N available in soil and that removed by the crop (Wagner-Riddle et al., 2007). The addition of N fertilizer stimulates nitrification and denitrification processes and thereby, increases both observed and simulated N_2O emissions (Abdalla et al., 2010; Abdalla et al., 2012). The significant differences between the simulated and observed daily N_2O fluxes peaks resulted in a somewhat poor correlation between the daily simulated and observed values. Generally, the field/ simulated N_2O peak emission events can account for approximately 50-90% of the yearly emissions (Parkin and Kaspar, 2006; Wolf et al., 2010; Abdalla et al., 2014). However, both the observed and simulated values do provide some insight into likely peaks and trends in N_2O flux under different N management regimes. The model imperfectly estimated the cumulative flux for the control treatment (RD = 42%) as a result of poor estimation of WFPS (%), soil nitrate and crop yield under the control. One of the disadvantages of the DNDC is that the model does not simulate negative N_2O flux values as in the observed flux and therefore, overestimated the simulated flux. Another disadvantage is that, the model under-estimated the observed WFPS (%) which is an important determinant of N_2O flux (Dobbie and Smith, 2001). The WFPS (%) is one of the key requirements for a reliable simulation of N_2O (Frolking et al., 1998), as changing its value may reduce the contribution of simulated nitrification/ denitrification processes (Li et al., 2001). Moreover, the high sensitivity of the DNDC model to rainfall events, SOC and temperature rendered the model less accurate since it simulated many higher N_2O peaks that were not observed in the field. Uncertainties in the observed values were also possible due to the limited number of field measurements (Parkin, 2008) as N_2O is released in pulses from soils to the atmosphere (Hastings et al., 2010) and peaks may appear for a maximum of few weeks only (Bell et al., 2012). Khalil et al. (2016)

reported that it is important to use a robust measurement protocol to get accurate validation of the DNDC model in response to different management practices.

In this study, the DNDC model generally overestimated the cumulative observed N_2O flux from the N treatments by an overall average of 13%. However, as the seasonal/ annual cumulative N_2O fluxes were calculated by the interpolation method, and due to the fact that the N_2O gas is characterized by episodic emissions, the observed cumulative emission could have high uncertainties. Ju et al. (2011) reported that a sampling frequency of 3 or 6 days resulted in an overestimation ranged from 112 to 228% in the total flux. According to Zhang et al. (2002), the present version of DNDC is qualified for incorporating crop residue in the soil and at the end of growing seasons. Residue turnover influences amounts of C and N added to the soil and thereby, N_2O emissions. Previous studies have also shown an increase in simulated N_2O flux due to the incorporation of cover crop residues into soils (Aulakh et al., 1984; Xiong et al., 2002; Sarkodie-Addo et al., 2003). They justified that by the extra energy available for denitrification, although provision of soil N through mineralisation of crop residues must also be considered.

4.2.2 Crop yields

The DNDC model estimated crop grain yield for all N treatments effectively. However, the model had difficulties in correctly estimating crop yield for the control treatment. This was due to significantly under-predicting of both soil nitrate and WFPS (%) for the control treatment. Additionally, the inability of the DNDC to correctly simulate the plant growth, although improved by calibration, was a potential source of yield reductions in the control treatment (Hu et al., 2017). Moreover, Abdalla et al. (2014) suggested improving the simulation of crop yield by developing the crop growth module to include degree days of phenology stages and radiation use efficiency for defining the growth curves for the crop. A new algorithm to the crop sub-model was introduced by Zhang et al. (2002) for the China-DNDC-online, and acts as an alternative approach to the empirical crop growth sub-model employed in DNDC (Li et al. 1994). Reasonable simulation of crop yield is of key importance to accurately predict N_2O emissions for process-based models of plant-soil systems.

4.2.3 Soil properties

The DNDC model effectively simulated soil temperature (0-5 cm depth) from the summer maize-winter wheat double cropping system with r^2 ranging from 0.96 to 0.97. This is comparable with the previously published studies of DNDC-temperature simulations under crop multiple cropping system carried by Cui et al. (2014), Uzoma et al. (2015) and Li et al. (2017). Cui et al. (2014) found r^2 ranged from 0.97 to 1.0, whilst Li et al. (2017) reported r^2 ranged from 0.89 to 0.97 between simulated and observed soil temperature for 0-5 cm and 0-10cm depth, respectively. The model successfully predicted observed soil temperature by tracing heat transfer between the different soil layers driven by soil heat capacity, temperature gradient and heat conductivity. Our study revealed that the present algorithm in DNDC is capable of correctly simulating soil temperature for double cropping system. This is important because the ability of the model to simulate soil temperature is essential for simulating GHG emissions, especially N_2O emissions. Soil temperature influences decomposition of soil organic matter and response of soil microorganisms to other perturbations, such as the amount of N fertilization and rainfall at the site (Wennman and Katterer, 2006). Likewise, accumulated soil temperature is the main driver behind plant growth in the DNDC model. Plant growth directly governs C and N contents and water in soils and, therefore, it is crucial to be simulated correctly (Hu et al., 2012).

The DNDC model simulated WFPS (%) for all N treatments satisfactorily but was less effective than that for simulating soil temperature (0-5 cm depth). The model under-estimated the WFPS (%) and this increased the uncertainties associated with N_2O simulations and resulted in poor fit with the observed flux (Wattenbach et al., 2010). The WFPS (%) determines if a soil is anaerobic or aerobic by influencing the concentration and transport of oxygen through the soil matrix (Song et al., 2019). Anaerobic conditions stimulate denitrification and result in much higher production rates of N_2O (Ussiri and Lal, 2012). In contrast, Kuang et al. (2019) suggested that higher WFPS (%) reduces N_2O emissions due to consumption and low gas diffusivity. Similar results for simulating WFPS (%) by DNDC in multiple and monoculture crops were reported in previous studies (e.g. Abdalla et al., 2014; Cui et al., 2014; Li et al., 2017). The range of r^2 between simulated and observed values reported in these previous studies was 0.1 to 0.6, compared to 0.4 to 0.5 found in this study. However, a previous study found that the underestimation of water dynamics by the DNDC, in a similar studies in North China plain, was due to the model uncertainty in estimating potential evapotranspiration (Kröbel et al., 2010). To further improve the simulation of WFPS (%) for double cropping system, the water module of DNDC needs to be further improved and any impact on the other submodules of the model should be considered.

The DNDC underestimated the magnitude of daily soil N (exchangeable NH_4^+ and NO_3^-) concentrations. Similar findings were showed by Abdalla et al. (2014) for a reduced tillage-cover crop experiment. The underestimation of WFPS (%) by DNDC, especially for the control treatment, could be one of the reasons behind this underestimation of daily soil N. The presence of two crops growing consecutively in the double cropping system increased the amount of C and N turnover from crop residues and made it difficult for the model to correctly simulate daily soil N. New features to quantify added C and N from crop residue are needed and the algorithms for simulating these multiple cropping systems in the double cropping system need to be improved.

5 Conclusions

In this study, the calibrated and evaluated DNDC model was able to effectively estimate cumulative N_2O flux and grain yields from the summer maize-winter wheat double cropping system. Conversely, the model generally underestimated daily soil N and WFPS (%) across all the N management regimes. The high sensitivity of the DNDC model to rainfall, SOC and temperature resulted in significant overestimation of N_2O peaks especially during the warm wet season. The DNDC model is weak in simulating the control treatment. To further improve the model’s performance, further future studies are needed to identify and resolve the existing problems especially with the control treatment.

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Tables

Table 1 Crop parameters used to calibrate the DNDC model for grain yield in each cropping season and simulated and observed grain yields.

Cropping season/ parameter	Grain	Leaf	Stem	Root	Simulated yield (t ha^{-1})	Observed yield (t ha^{-1})
Summer maize 2012						
Maximum biomass production (kg C ha^{-1}y^{-1})	3850	1694	1694	462	3.9	3.9
Biomass fraction	0.5	0.22	0.22	0.06		
Biomass C/N ratio	50	80	80	80		
Thermal degree days	2550					
Water demand (g water/g DM)	150					
Optimum temperature (°C)	30					
Winter wheat 2012-2013						
Maximum biomass production (kg C ha^{-1}y^{-1})	3300	1732	1732	1485	3.0	3.0
Biomass fraction	0.4	0.21	0.21	0.18		
Biomass C/N ratio	40	95	95	95		
Thermal degree days	1300					
Water demand (g water/g DM)	200					
Optimum temperature (°C)	22					
Summer maize 2013						
Maximum biomass production (kg C ha^{-1}y^{-1})	3550	1562	1562	462	3.5	3.5
Biomass fraction	0.5	0.22	0.22	0.06		
Biomass C/N ratio	50	80	80	80		
Thermal degree days	2550					
Water demand (g water/g DM)	150					
Optimum temperature (°C)	30					
Winter wheat 2013-2014						
Maximum biomass production (kg C ha^{-1}y^{-1})	3300	1540	1540	953	2.8	2.8
Biomass fraction	0.45	0.21	0.21	0.13		
Biomass C/N ratio	40	95	95	95		
Thermal degree days	1300					
Water demand (g water/g DM)	200					
Optimum temperature (°C)	22					

Table 2 Statistical evaluations of simulated daily soil temperature, WFPS, nitrate and cumulative N_2O fluxes compared with the observed values under different N management of summer maize -winter wheat double cropping system from 2012 to 2014.

Treatment/parameter	Observed	Simulated	RD (%)	RMSE	nRMSE (%)	EF	d
Control							
Average daily soil temperature (ºC)	16.3	20.0	23	4.1	25	0.89	0.89
Average daily WFPS (%)	57.0	13.6	-76	42	74	<0	0.40
Average daily soil N (kg N ha^{-1})	1.1	0.1	-91	0.54	4	0.58	0.58
N_2O emissions	1.1	1.5 (1.8)*	42	0.55	4	<0	0.10
Conventional N							
Average daily soil temperature (ºC)	16.3	20.1	23	4.2	26	0.79	0.89
Average daily WFPS (%)	54.7	20.7	-62	12.9	24	<0	0.43
Average daily soil N (kg N ha^{-1})	87.7	69.5	-21	2.39	3	0.11	0.75
N_2O emissions	12.0	10.4 (5.5)	-13	2.59	16	<0	0.50
Optimal N							
Average daily soil temperature (ºC)	16.3	20.0	23	4.1	25	0.96	0.97
Average daily WFPS (%)	55.0	20.2	-63	37.4	67	0.10	0.51
Average daily soil N (kg N ha^{-1})	49.7	28.6	-42	1.32	2	<0	0.57
N_2O emissions	6.9	7.9 (3.5)	16	1.9	20	<0	0.29
1.3*Optimal N							
Average daily soil temperature (ºC)	16.3	20.0	23	4.1	25	0.96	0.97
Average daily WFPS (%)	55.0	20.1	-63	37.0	67	0.10	0.75
Average daily soil N (kg N ha^{-1})	6.3	5.1	-19	0.27	4	0.02	0.74
N_2O emissions	8.6	9.5 (4.6)	10	2.18	20	<0	0.29

* The values between brackets represent the model results before calibration.

Table 3 Comparisons between the DNDC- simulated and observed annual grain yields (t ha^{-1}) (2012-2014) of the summer maize - winter wheat double cropping system before and after the DNDC model calibration.

Treatment	Grown seasonal crop	Season/ Year	Observed yield	Simulated yield (before)	Simulated yield (after)	RD (%; before)	RD (%; after)
Control	Summer maize	2012	6.7	0.2	4.8	-97	-30
	Summer maize	2013	5.2	0.4	3.0	-92	-40
Conventional N	Summer maize	2012	10.2	12.0	9.8	18	-5
	Summer maize	2013	9.5	11.4	9.0	20	-5
Optimal N	Summer maize	2012	9.5	10.5	9.8	11	7
	Summer maize	2013	9.7	10.0	9.0	03	-7
1.3* Optimal N	Summer maize	2012	10.4	11.1	9.7	07	-7
	Summer maize	2013	9.5	10.0	8.9	05	-6
Control	Winter wheat	2013	2.3	0.3	1.1	-87	-50
	Winter wheat	2014	2.3	0.4	0.9	-83	-60
Conventional N	Winter wheat	2013	8.2	13.0	8.0	59	-2
	Winter wheat	2014	7.9	5.8	6.3	-27	-21
Optimal N	Winter wheat	2013	8.0	8.8	8.0	11	0
	Winter wheat	2014	7.8	4.5	8.3	-42	6
1.3* Optimal N	Winter wheat	2013	8.0	11.3	8.0	41	0
	Winter wheat	2014	8.1	5.1	8.2	-37	2

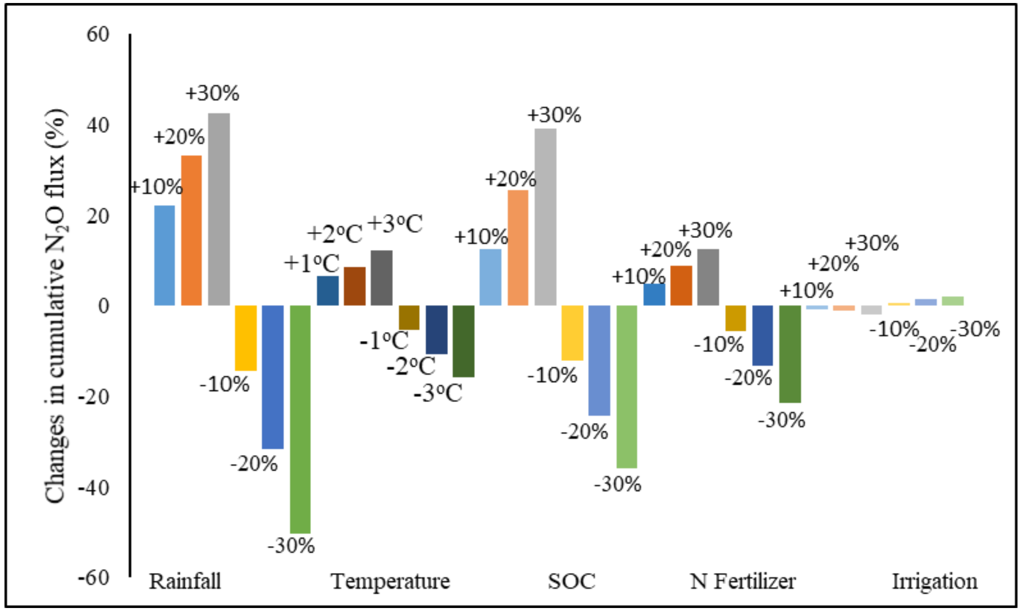
Figure captions

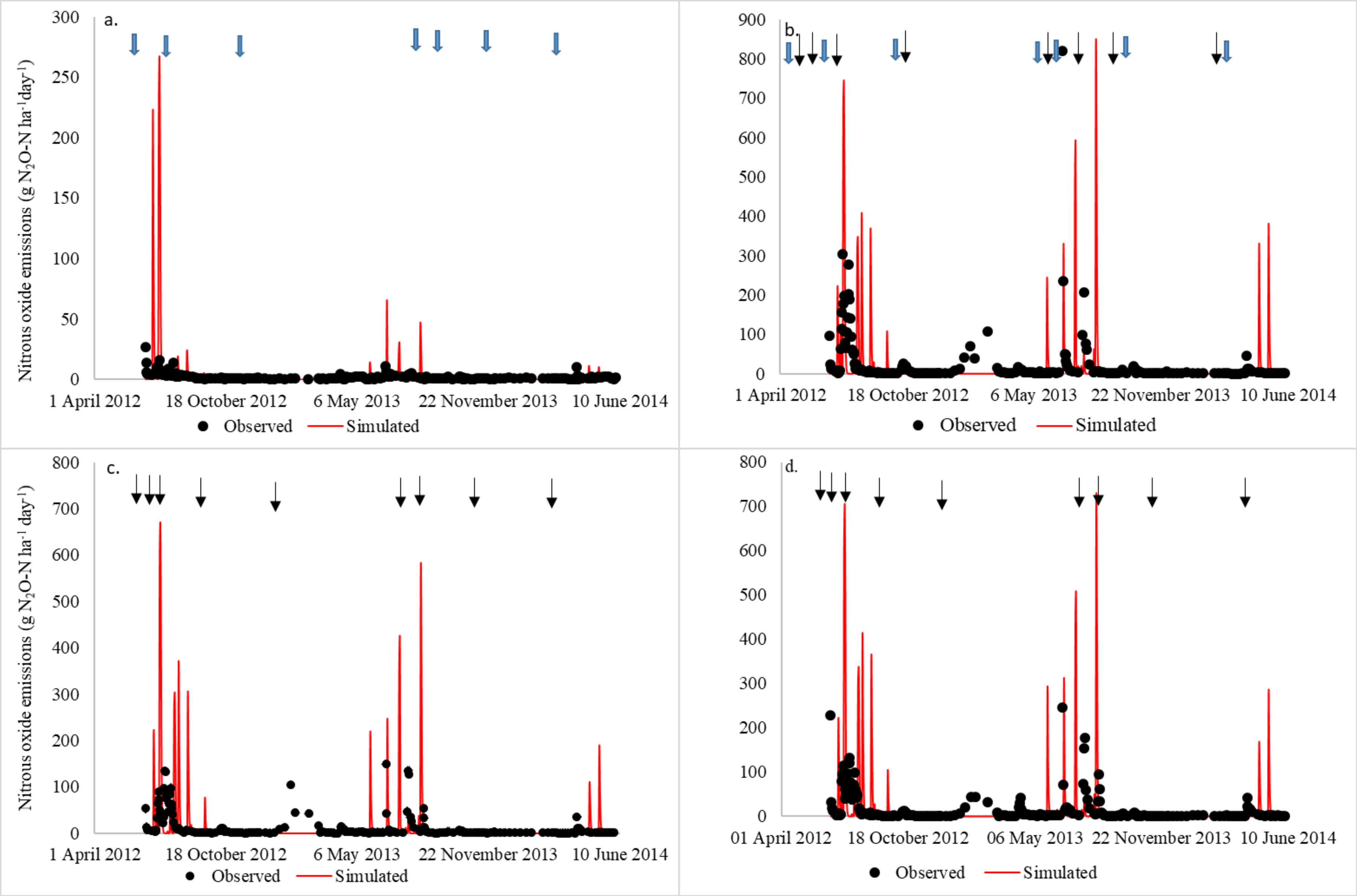
Fig. 1 Sensitivity analysis of the DNDC model to changes in the input parameters (i.e. daily precipitation, daily air temperature, soil organic C (SOC), applied N fertilizer and water irrigation).

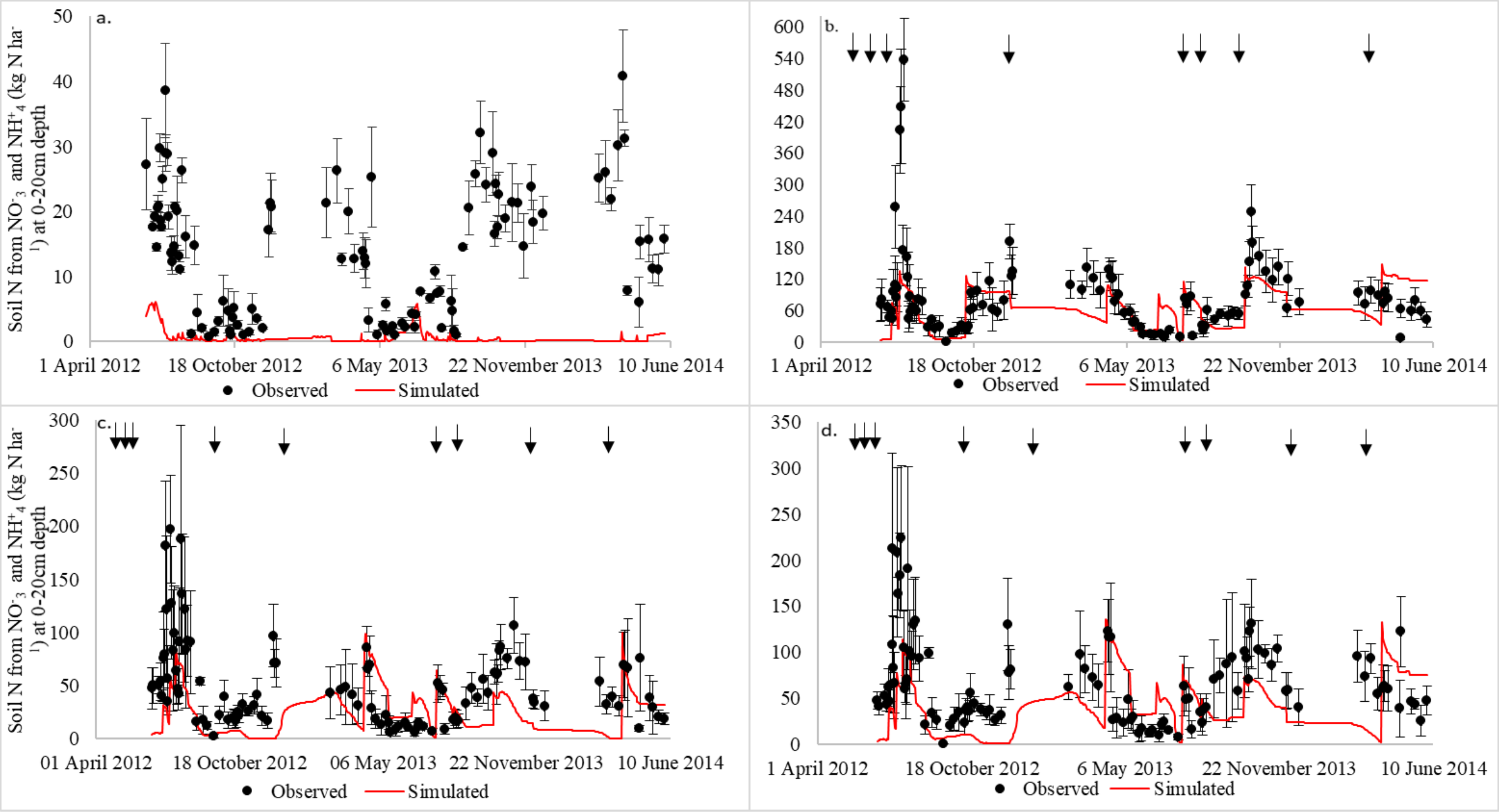
Fig. 2 Comparisons between DNDC- model-simulated (red lines) and field observed (●) daily N_2O fluxes from the control (a), conventional N (b), optimal N (c), and 1.3*optimal N (d) fertilizer application rate over the experiment period of the maize-wheat double cropping system (2012-2014). Black arrows show the date of N fertilizer application and blue arrows show the date of water irrigation. (Error bars for observed values are ± standard error).

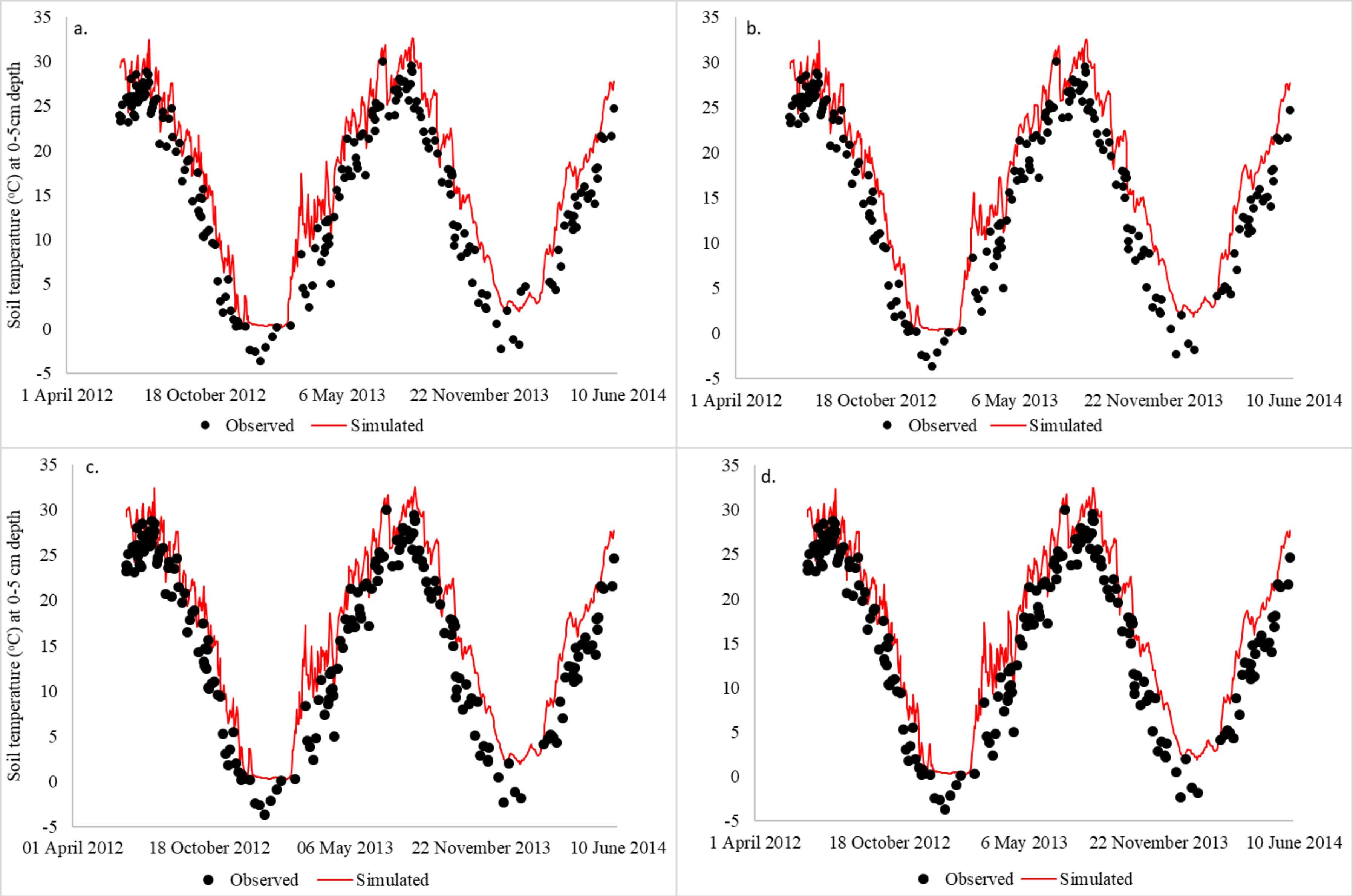
Fig. 3 Comparisons between the DNDC-model- simulated (line) and field observed (●) soil nitrate plus ammonium (kg N ha^{-1}) at 0-20cm depth from the control (a; $r^2 = 0.15$), conventional (b; $r^2 = 0.17$), optimal N (c; $r^2 = 0.15$) and 1.3*optimal N (d; $r^2 = 0.11$). Arrows show times of fertilizer application. (Error bars for observed values are ± standard error).

Fig. 4 Comparisons between the DNDC- model- simulated and field observed daily soil temperature (^{o}C) at 0-5cm depth; for control (a), conventional N (b), optimal N (c) and 1.3* optimal N (d).


Changes in cumulative N$_2$O flux (%)
60
40
20
0
-20
-40
-60
+10%
+20%
+30%
-10%
-20%
-30%
+1°C
+2°C
+3°C
-1°C
-2°C
-3°C
+10%
+20%
+30%
-10%
-20%
-30%
+10%
+20%
+30%
-10%
-20%
-30%
+10%
+20%
+30%
-10%
-20%
-30%
Rainfall
Temperature
SOC
N Fertilizer
Irrigation


a.
Nitrous oxide emissions (g N_2O-N $ha^{-1}day^{-1}$)
0
50
100
150
200
250
300
1 April 2012
18 October 2012
6 May 2013
22 November 2013
10 June 2014
● Observed
Simulated
b.
0
100
200
300
400
500
600
700
800
900
1 April 2012
18 October 2012
6 May 2013
22 November 2013
10 June 2014
● Observed
Simulated
c.
Nitrous oxide emissions (g N_2O-N ha^{-1} day^{-1})
0
100
200
300
400
500
600
700
800
1 April 2012
18 October 2012
6 May 2013
22 November 2013
10 June 2014
● Observed
Simulated
d.
0
100
200
300
400
500
600
700
800
01 April 2012
18 October 2012
06 May 2013
22 November 2013
10 June 2014
● Observed
Simulated


a.
b.
c.
d.
Soil N from NO$^{-}_{3}$ and NH$^{+}_{4}$ (kg N ha^{-1}) at 0-20cm depth
50
40
30
20
10
0
600
540
480
420
360
300
240
180
120
60
0
300
250
200
150
100
50
0
350
300
250
200
150
100
50
0
1 April 2012
01 April 2012
18 October 2012
6 May 2013
06 May 2013
22 November 2013
10 June 2014
Observed
Simulated


a.
b.
c.
d.
Soil temperature (°C) at 0-5cm depth
Soil temperature (°C) at 0-5 cm depth
35
30
25
20
15
10
5
0
-5
1 April 2012
01 April 2012
18 October 2012
6 May 2013
06 May 2013
22 November 2013
10 June 2014
● Observed
Simulated

Supplementary Materials

Table S1 Nitrogen fertilizer application rates (kg N ha^{-1}) and irrigation (mm) at the different N fertilizer management during the experimental period 2012-2014

Growing season	Date	Control	Conventional N	Optimal N	1.3*optimal N	0.7*optimal N	Irrigation rate
2012 maize	17 June	0	-	-	-	-	90
	3 July	0	100[a]	45[a]	59[a]	32[a]	-
	13 July	0	150[b]	69[b]	89[b]	48[b]	-
	21 July	0	0	58[a]	75[a]	40[a]	-
	Total	0	250	172	223	120	90
2012-2013 wheat	8 Oct. 2012	0	150[c]	50[c]	65[c]	35[c]	
	5 Dec. 2012	0	0		0	0	75
	10 Apr. 2013	0	150[b]	139[b]	181[b]	97[b]	70
	13 May 2013	0	0		0	0	90
	Total	0	300	189	246	132	235
2013 maize	16 June	0	100[c]	45[c]	59[c]	32[c]	-
	18 June	0	-	-	-	-	75
	19 July	0	150[b]	90[b]	117[b]	63[b]	
	13 August	0	0	30[b]	39[b]	21[b]	-
	Total	0	250	165	215	116	75
2013-2013 wheat	7 Oct. 2013	0	150[c]	50[c]	65[c]	35[c]	
	1 Dec. 2013	0	0	0	0	0	75
	4 Apr. 2014	0	150[b]	127	165[b]	89[b]	90
	Total	0	300	177	230	124	165

Letters a-c represent the N application method: [a]= Band application followed by soil covering; [b]= Surface broadcast; [c]= incorporating surface applied N into soil.

Supplementary Figures

Figure captions

Fig. S1 Average air temperature (^{o}C) and daily precipitation (mm) at the experimental site during the study period of 2012-2014.

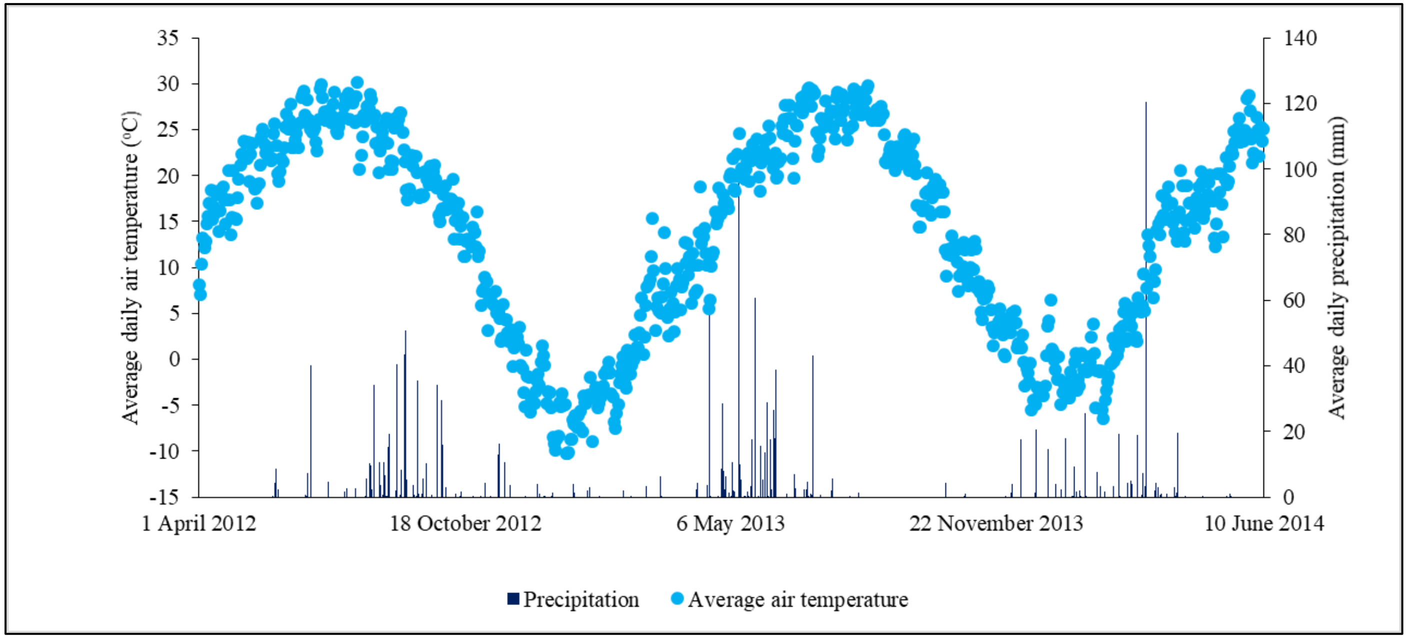
Fig. S2: A 1:1 relationship between the DNDC simulated and field observed cumulative N_2O emissions from the maize-wheat double cropping system ($y = 0.99x$ and $r^2 = 0.91$).

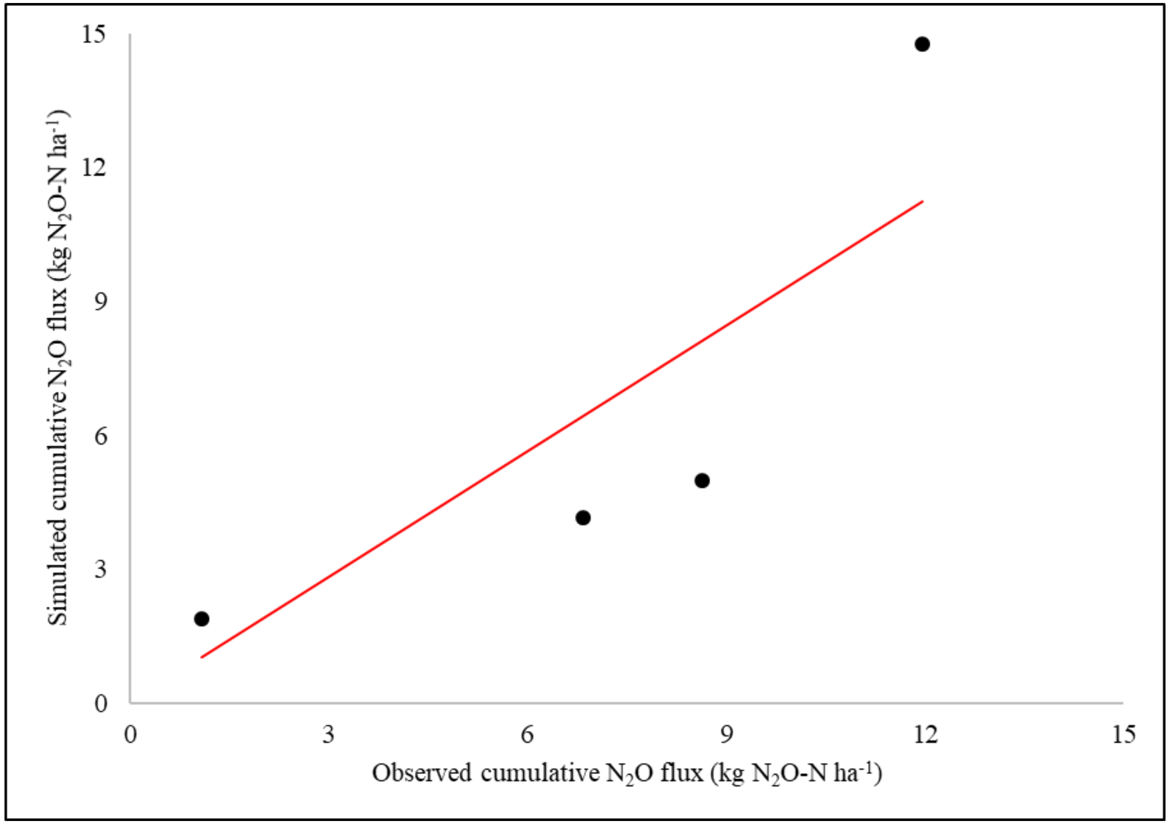
Fig. S3: 1:1 relationships between DNDC-simulated and field observed grain yields; for maize/wheat combination (a; $r^2 = 0.91$), maize (b; $r^2= 0.89$) and wheat (c; $r^2= 0.92$).

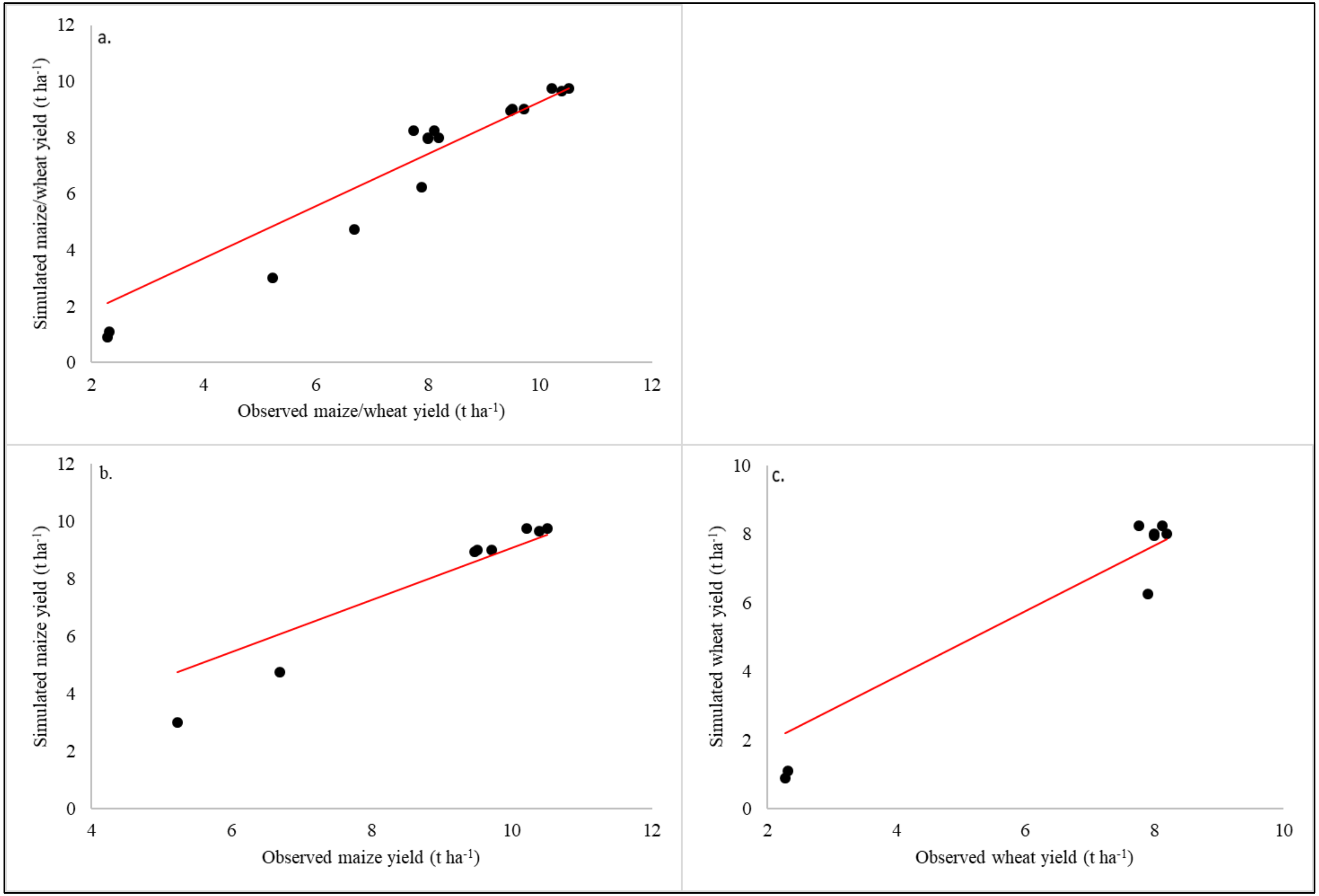
Fig. S4: 1:1 relationships between daily DNDC-simulated and field observed water filled pore space (WFPS; %) at 0-20 cm depth; for control (a; $r^2 = 0.30$), conventional N (b; $r^2= 0.37$), optimal N (c; $r^2= 0.31$) and 1.3* optimal N (d; $r^2 = 0.37$). (Error bars for observed values are ± standard error).

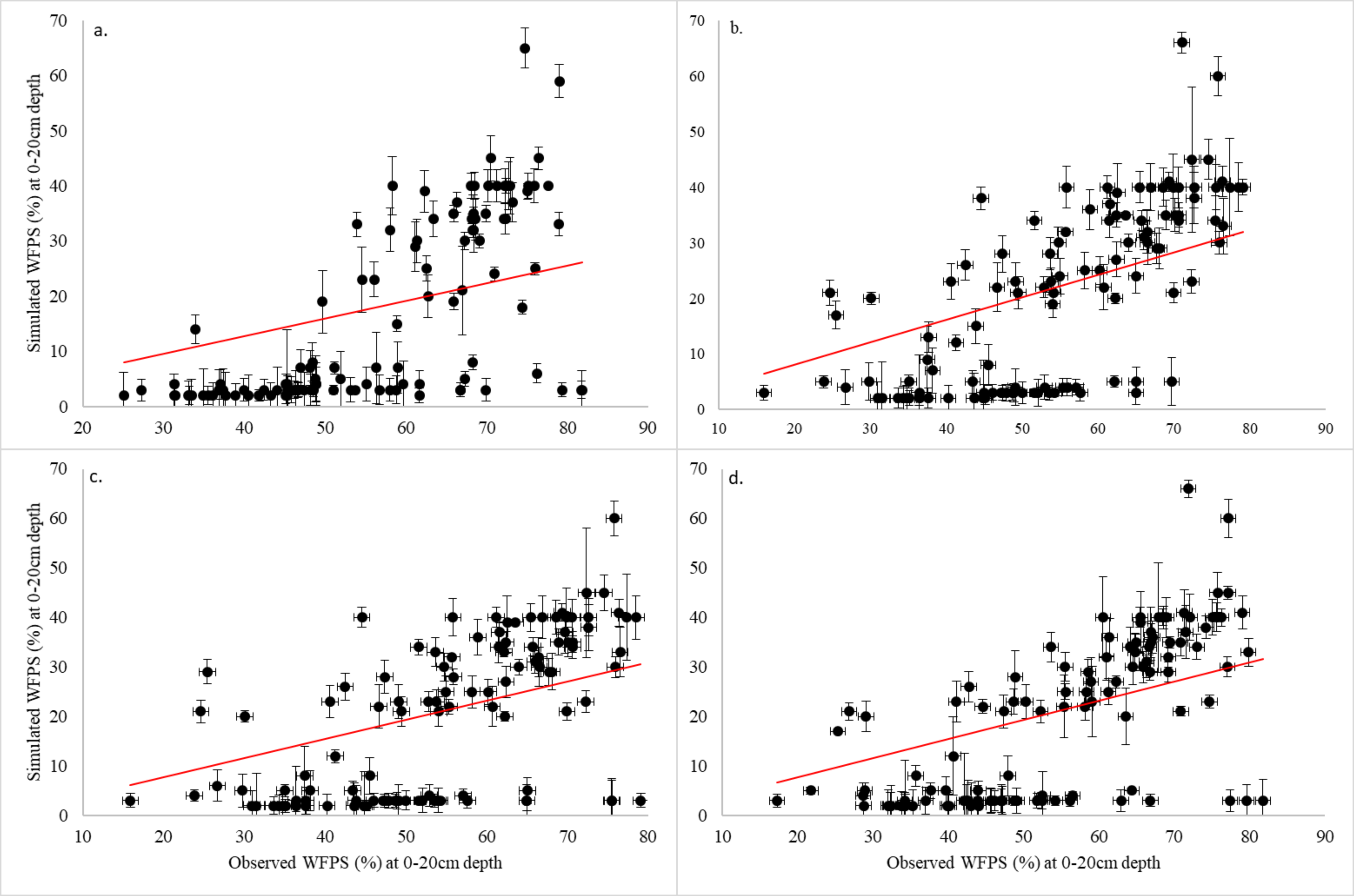
Fig. S5: A 1:1 relationship between the DNDC simulated and field observed cumulative soil N for the maize-wheat double cropping system ($y= 0.74x$; $r^2 = 0.97$).

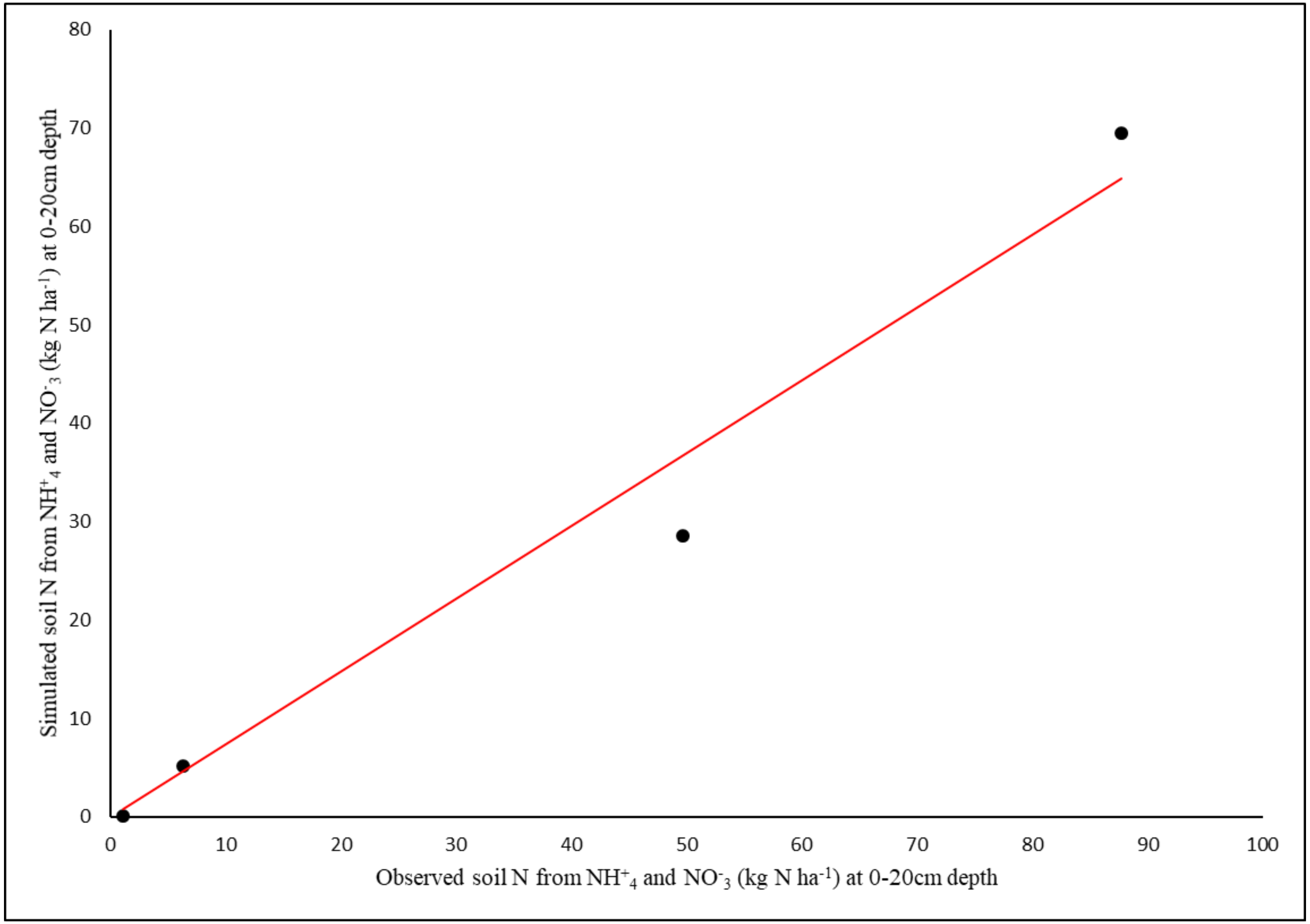
Fig. S6: 1:1 relationships between daily DNDC-simulated and field observed soil temperature (^{o}C) at 0-5 cm depth; for control (a; $r^2 = 0.89$), conventional N (b; $r^2= 0.88$), optimal N (c; $r^2= 0.88$) and 1.3* optimal N (d; $r^2 = 0.88$).

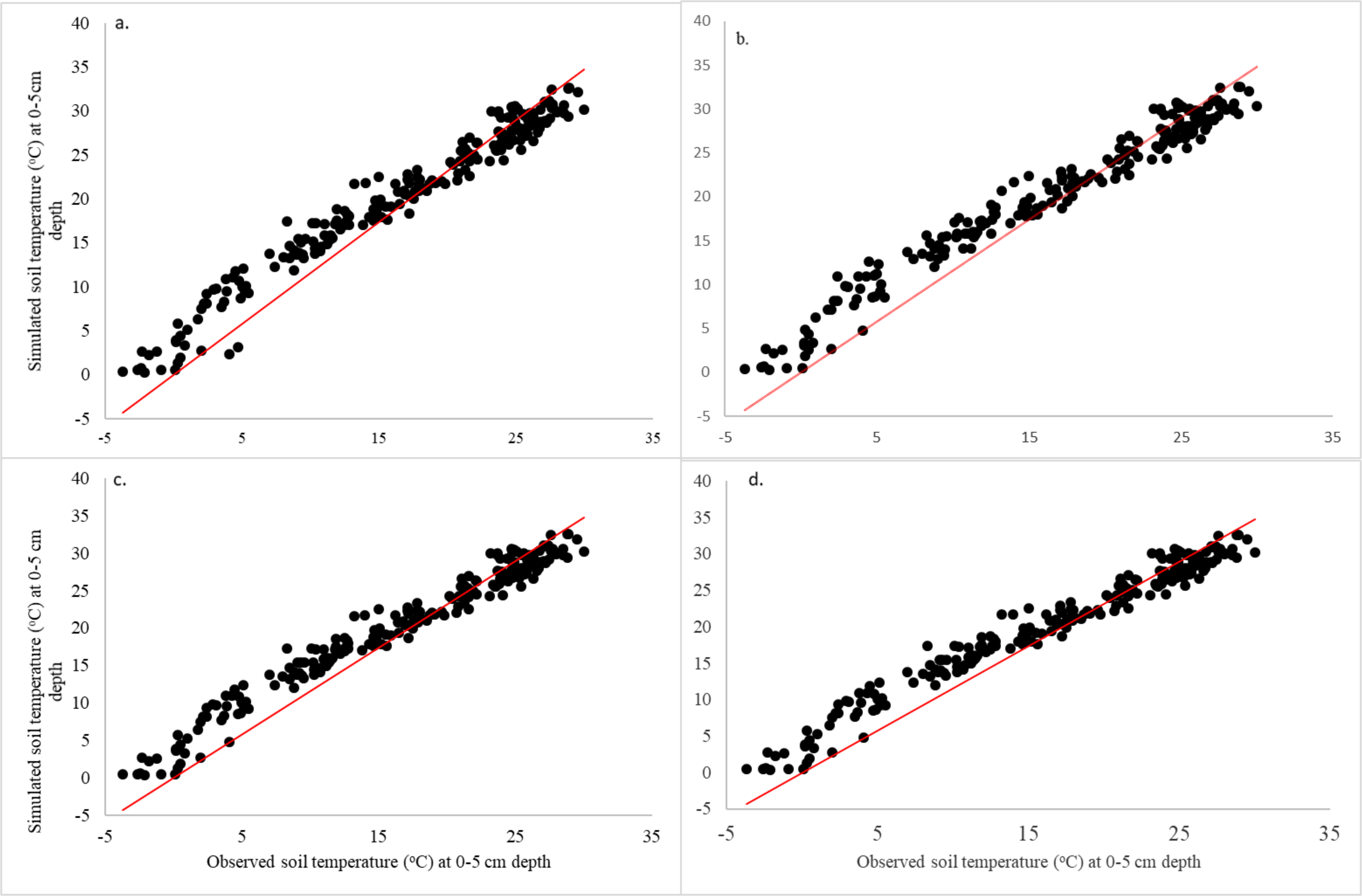

Average daily air temperature (°C)
35
30
25
20
15
10
5
0
-5
-10
-15
Average daily precipitation (mm)
140
120
100
80
60
40
20
0
1 April 2012
18 October 2012
6 May 2013
22 November 2013
10 June 2014
■ Precipitation
● Average air temperature


Simulated cumulative N_2O flux (kg N_2O-N ha^{-1})
Observed cumulative N_2O flux (kg N_2O-N ha^{-1})
0
3
6
9
12
15
0
3
6
9
12
15


a.
Simulated maize/wheat yield (t ha-1)
Observed maize/wheat yield (t ha-1)
0
2
4
6
8
10
12
2
4
6
8
10
12
b.
Simulated maize yield (t ha-1)
Observed maize yield (t ha-1)
0
2
4
6
8
10
12
4
6
8
10
12
c.
Simulated wheat yield (t ha-1)
Observed wheat yield (t ha-1)
0
2
4
6
8
10
2
4
6
8
10


a.
b.
c.
d.
Simulated WFPS (%) at 0-20cm depth
Observed WFPS (%) at 0-20cm depth
0
10
20
30
40
50
60
70
80
90


0
10
20
30
40
50
60
70
80
0
10
20
30
40
50
60
70
80
90
100
Simulated soil N from NH^+_4 and NO^-_3 (kg N ha^{-1}) at 0-20cm depth
Observed soil N from NH^+_4 and NO^-_3 (kg N ha^{-1}) at 0-20cm depth


a.
b.
c.
d.
Simulated soil temperature (ºC) at 0-5cm depth
Simulated soil temperature (ºC) at 0-5 cm depth
Observed soil temperature (ºC) at 0-5 cm depth
Observed soil temperature (ºC) at 0-5 cm depth
40
35
30
25
20
15
10
5
0
-5
-5
5
15
25
35