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# Estimation of greenhouse gases ($N_2O$, $CH_4$ and $CO_2$) from *no-till* cropland under increased temperature and altered precipitation regime: a DAYCENT model approach

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ABSTRACT

Greenhouse gas (GHG) emissions play an important role in regulating the Earth surface temperature. GHG emissions from soils are sensitive to climate change and land management practices. According to general circulation model (GCM) predictions, the Earth will experience a combination of increased temperature and altered precipitation regimes which may result in an increase or a decrease of GHG exchange. The effect of climate change on GHG emissions can be examined through both experiments and by applying process-based models, which have become more popular. The performance of those models can be improved significantly by appropriate calibration procedures. The objectives of this study are to: (i) calibrate the DAYCENT model using advance parameter estimation (PEST) software and to (ii) examine simulated GHG dynamics at daily and seasonal time-scales under a climate change scenario of increased temperature (2 °C) and a precipitation regime change where 40% of precipitation during the dry season was redistributed to the wet season. The algorithmic calibration improved the model performance by reducing the sum of weighted squared residual differences by up to 223% (decreased from 1635 to 505 g $N_2O$-N $ha^{-1}$ $d^{-1}$) for $N_2O$ and 22% (decreased from 623 to 507% WFPS) for water filled pore space (WFPS) simulation results. In the altered climate scenario, total $N_2O$ and $CO_2$ fluxes decreased by 9% (from 2.31 to 2.10 kg $N_2O$-N $ha^{-1}$ $yr^{-1}$) and 38% (from 1134.08 to 699.56 kg $CO_2$ $ha^{-1}$ $yr^{-1}$) respectively, whereas $CH_4$ fluxes increased by 10% (from 1.62 to 1.80 kg $CH_4$ $ha^{-1}$ $yr^{-1}$). Our results show a larger impact of altered climate on $CO_2$ as compared to $N_2O$ and $CH_4$ emissions. The main difference in all GHG emissions was observed in summer period due to drought conditions created by reduced precipitation and increased temperatures. However, the GHG dynamics can also be attributed to no-till practices which play an important role in changing the soil moisture conditions for aerobic and anaerobic microsites. These results are based on a process-based model, therefore, we suggest performing experimental studies to examine the GHG emissions under increased temperature and especially under altered precipitation regimes.



## 1. Introduction

Greenhouse gas (GHG) exchange between soils and the atmosphere is an important contributing factor to global climate change. The main GHGs from agricultural systems are nitrous oxide ($N_2O$), methane ($CH_4$) and carbon dioxide ($CO_2$) which play an important role in regulating Earth surface temperature. Nitrous oxide is produced by microbial transformation (nitrification and denitrification) of nitrogen (N) compounds in soils, whereas $CH_4$ is generated when organic material is decomposed in oxygen deprived conditions which is especially the case for flooded land (Goulding et al., 1995). Carbon dioxide is lost from agricultural soils by respiration and decomposition of soil organic matter (SOM). According to USEPA (2011), agricultural systems contributed the equivalents of 503 Tg (1Tg = $10^{12}$ g) $CO_2$ in 2008 which is only surpassed by electric generation, transportation and industry. Globally the U.S. is the second highest emitter of GHG after China and followed by the European Union, India and Russia.

Based on general circulation models (GCM) projections, most parts of the globe are predicted to face a combination of atmospheric warming (1.5–4.5 °C) and modified precipitation regimes characterized by a reduced number of large events and a shift from summer to spring distribution during this 21st century (Sillmann et al., 2013; Volder et al., 2013). The occurrence of warmer temperatures and greater evapotranspiration coupled with a decrease in summer precipitation will collectively intensify summer droughts (Pope et al., 2000; MacCracken et al.,

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2003). Variations in climatic factors strongly affect the GHG balance in agricultural systems. For example, temperature and precipitation change can alter the carbon (C) storage capacity and GHG fluxes from soil through effects on net primary production (NPP), C and N inputs into the soil, SOM decomposition rates and N cycling. Precipitation determines the water filled pore space (WFPS) in soil which impacts GHG fluxes by influencing the oxygen status of the soil (Rafique et al., 2011a, 2011b).

Agricultural GHG emissions are complex and heterogeneous due to the combined effect of meteorological drivers as well as land management and soil properties (Rafique et al., 2011a). For example, by enhancing C sequestration, reduced tillage practices are considered a good GHG mitigation strategy in cropland (Lal, 2004). The understanding of GHG exchange between agricultural ecosystems and the atmosphere can be improved through direct observations and experiments, as well as through modeling studies. In the last few decades modeling approaches have become popular compared to experimental studies. Process based ecosystem models such as DAYCENT (Del Grosso et al., 2005), CENTURY (Parton et al., 1998), DNDC (Li et al., 2000), EPIC (Wang, 2005) and RothC (Xu et al., 2011) have become integral tools for extrapolating local observations in addition to testing different hypotheses of ecosystem response to climate changes, nutrient variability and land management (Rafique et al., 2011b). Models vary in their specific goals and approaches, but their central role is to provide a better understanding of the mechanism responsible for GHG emissions and C turnover. Without a doubt, the precision of these models strongly depends on their proper parameterization. If such models are calibrated and validated properly against existing data from various sites, they can be used to build GHG inventories on various temporal and spatial scales. An algorithmic calibration has proven to be superior over manual calibration of the models. An algorithmic calibration is also called inverse modeling as it integrates experimental data into the model and provides a best estimate of the parameters by reducing residual differences between modeled and observed values based on mathematical and statistical principles (Rafique et al., 2013).

Specific objectives of this study are: to (i) calibrate the DAYCENT model using advance parameter estimation (PEST) software and to (ii) examine simulated GHG dynamics at daily and seasonal time-scales under a climate change scenario of increased temperature (2 °C) and an altered precipitation regime.

## 2. Methods

### 2.1. Experimental data

For this analysis of the altered climate change scenario, we used $N_2O$ flux and WFPS data measured in the year 2003 from corn/soybean fields located at the Agronomy Research Farms (latitude 42.02 and longitude −93.77) of Iowa State University, Iowa. This site has been under a no-till (NT) system with controlled traffic since 1995. For the year 2003, an annual rainfall of 89.06 cm was recorded with an average air temperature of 9.76 °C. The temporal variation of measured air temperature along with precipitation is shown in Fig. 1. Nitrogen fertilizer was applied at a rate of 13 kg N $ha^{-1}$ at planting time (early May) and 202 kg N $ha^{-1}$ 38 days after planting. The crop was harvested in early November (Fig. 3). Soil samples were collected at 0–30 cm for physical and chemical analysis. Daily precipitation and average air and soil temperatures were taken from a meteorological station (Herzmann, 2004) located 0.5 km west of the study area. Detailed description of $N_2O$ flux chamber measurements, soil properties and field management (e.g. planting and harvesting of crops) has been previously described in Parkin and Kaspar (2006).

### 2.2. Model setup and parameterization

In this study the DAYCENT (version 4.5) model was utilized at a daily time-step to simulate environmental processes such as trace gas fluxes (Parton et al., 1987) which cannot be sufficiently simulated at the longer time-steps possible with the CENTURY terrestrial ecosystem model. Model inputs are: daily precipitation, maximum and minimum daily temperature, vegetation type, soil texture and historical land use. The DAYCENT model consists of several submodels e.g. soil water content, SOM decomposition, nutrient mineralization, plant growth, N gas production and $CH_4$ oxidation. The C and N turnover rates are determined by the size of the respective pools, C/N ratio, water/temperature factors and lignin content of the material. Net primary productivity (NPP) and C allocation are determined by the plant phenology, nutrient availability and water/temperature stress. The decomposition processes represented in the submodel are controlled by the substrate availability, substrate quality, soil water content and temperature. $N_2O$ gas emissions are a function of soil $NH_4^+$ and $NO_3^-$ concentrations, soil moisture, temperature, texture and C availability. Soil $NH_4^+$ and $NO_3^-$ concentrations are collectively determined by N mineralization, N fixation, N fertilizations and N deposition. $NO_3^-$ is distributed throughout the soil profile while $NH_4^+$ is modeled only for the top 15 cm layer. The DAYCENT model also considers soil and plant N fixation. Soil N fixation is controlled as a function of the mineral N to labile P ratio or as a linear function of annual precipitation. Similarly, the plant N fixation only occurs where there is insufficient mineral N to satisfy the plant N requirement and is dependent on plant type and growth rate. The model outputs are highly dependent on historical land use which impacts the SOC and mineral N levels in the soil. For this study, to properly initialize the C and N pools we simulated a series of temperate tall grass, low yield wheat, low yield corn, clover grass, medium yield corn, soybean and weeds from year 1 until 2002. The DAYCENT model has the ability to generate long term statistical (precipitation means, standard deviation, skewness values, minimum temperature, means and maximum temperature) weather data based on the present limited weather data.

DAYCENT was parameterized carefully using the model-independent parameter estimation software, PEST, which is a public-domain software used for highly parameterized model calibration based on linear regression. PEST implements a gradient-based optimization approach to linearize nonlinear problems by computing the Jacobian matrix of sensitivities of model observations to parameters. The PEST software interacts with DAYCENT by modifying model inputs, running the model and evaluating model outputs until they reach convergence. The singular value decomposition (SVD) was applied in PEST to get numerical stability. The SVD was also combined with a reduction of parameters by disregarding the parameters with low sensitivity (Doherty, 2010). During the calibration process, PEST first reads the essential information such as parameters, observed data and regularization constraints required for execution process. In the first iteration, DAYCENT uses the current parameter values. In the end of first simulation, PEST extracts the model outputs from the DAYCENT model output files for a second iteration. PEST calls DAYCENT repeatedly, perturbing one parameter at a time, to adjust the parameter values. This process of iteration continues until the objective function is achieved. The algorithmic calibration method has been previously explained by Rafique et al. (2013).

The $N_2O$ flux and WFPS data were used to calibrate the model as these two measurements along with net primary productivity (NPP) are considered important factors for obtaining better estimates of modeled GHG. WFPS is important for determining the soil moisture conditions which directly control the soil microbial activities resulting in GHG fluxes. It is necessary to optimize $N_2O$ emissions by tuning several parameters in the DAYCENT model which differs from other GHGs (Del Grosso et al., 2000). However, $CH_4$ and $CO_2$ are strongly dependent on the soil properties, climatic conditions and NPP values. According to the DAYCENT developer (personal communication with Cindy Keough in Colorado State University), if we calibrate the model for $N_2O$ flux, WFPS along with correct output of NPP, the other GHG outputs can be considered reliable. Therefore, in this particular study the model calibration was carried out using $N_2O$ flux and WFPS data. The modeled NPP was compared with the average observed values in this study (data

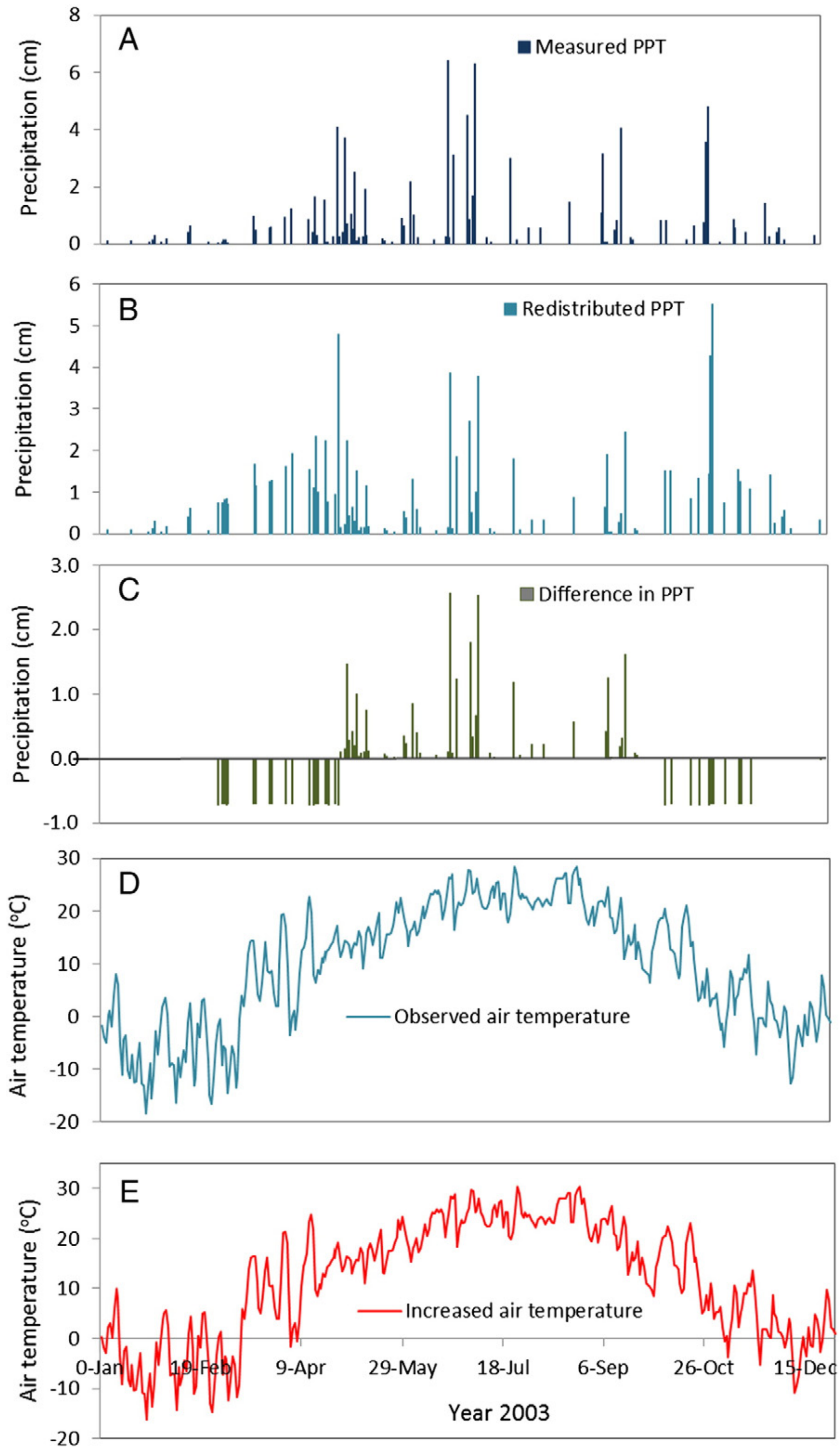


**Fig. 1.** (A) Daily observed precipitation, (B) daily precipitation used in climate scenario analysis, (C) difference between two precipitation regimes (from A and B), (D) daily mean air temperature observed at study site and (E) daily mean air temperature used in climate scenario analysis. PPT stands for precipitation.

not shown). The first step in the parameterization of the model was to determine the most sensitive parameters which strongly affect the $N_2O$ fluxes and WFPS (Rafique et al., 2013) outputs. The most sensitive parameters which influence the $N_2O$ and WFPS outputs were present in submodels: soil water, nitrification/denitrification, SOM, and crop production. Soil properties were taken from the field observations and are considered as basic control over GHG fluxes. Sensitivity analysis for 140 parameters was carried out starting from model developer-recommended default parameter values. The simulation results produced from default parameter values are called as "default simulation". Then, we used the 43 most sensitive parameters (with reference to $N_2O$ and WFPS outputs) and optimized them to run DAYCENT/PEST in calibration mode. The results obtained from calibration mode are called a "cold simulation" which serves as a base line to determine the effect of climate warming and precipitation regime changes. Cold simulation results were compared with default simulation to check the model improvement. Calibration performance was determined using the well-established statistical criteria of sum of weighted squared residuals (SWSR) and coefficient of determination.

### 2.3. Altered precipitation and warming scenario

The main tools we use for making scientific projections are process based models. In this study we used the DAYCENT model to examine the effect of potential future: (1) increase in air temperature and (2) altered precipitation regimes on GHG fluxes. For the scenario, air temperature was increased by 2 °C. In the precipitation regime shift, the dry phase precipitation (May to September) was reduced by 40% by subtracting this amount from each event and evenly distributing it to rainfall events of the wet phase of the year (March, April, October and November). This precipitation scenario also considers the reduced number of heavy rain events from the dry period. The total amount of precipitation along with number and timing of events was not changed. This temperature increase and precipitation redistribution will create arbitrary drought conditions during the dry period which are probable in the future (Volder et al., 2013). In this study simulated results obtained under scenario conditions are called “manipulated” results which were compared with “cold simulations” to examine the impact of increased temperature and precipitation redistribution. Then the seasonal fluxes were quantified in each of the four seasons of spring (Feb, Mar, Apr), summer (May, Jun, Jul), autumn (Aug, Sep, Oct) and winter (Nov, Dec, Jan). The increased temperature and redistributed precipitation along with difference between two precipitation regimes is shown in Fig. 1.

## 3. Results

### 3.1. Model calibration

Sensitivity analysis proved to be an important step in determining the most important parameters influencing the $N_2O$ fluxes and WFPS. The simulated $N_2O$ fluxes and WFPS were found to be most sensitive to 43 parameters out of 140. Other parameters have less or no effect on the model performance during the calibration process. The most sensitive parameters influencing $N_2O$ and WFPS results include *rcestr(1)*, *nit_amnt*, *fleach(3)* and *epnfs(2)* each of which showed sensitivities larger than 2.0. The *rcestr(1)* parameter determines the C/N ratio of structural material, while *nit_amnt* explains the daily nitrification amount occurring in soil. Similarly, *fleach(3)* is denoted as the leaching fraction multiplier to compute the fraction of N leached within or out of the soil. In remaining parameters, 8 parameters showed sensitivity greater than 1.0 followed by all others. The *damrmn* parameter was not found to be in the group of most sensitive parameters although it seems an important control on the direct absorption of N in plant residue. The parameters used in the calibration procedure along with their starting, lower, upper and optimized values are ranked (based on scaled sensitivity) in descending order in Table 1. The detailed description of the parameters is given in Appendix 1.

The parameter sensitivity in PEST is estimated using a finite difference approximation.

$$\frac{\partial y}{\partial p} = \frac{y(p+\nabla p) - y(p)}{\nabla p}$$

Where $\frac{\partial y}{\partial p}$ is the sensitivity of the modeled output (y) to a parameter (p). The combination of parameters and observations result in an NPAR × NOBS Jacobean sensitivity matrix which is used in Gauss-Marquardt-Levenberg (GLM) algorithm for regressions calculations.

$$J_{ij} = \frac{\partial_{yi}}{\partial_{pj}}$$

Where $i = 1$ to NOBS and $J = 1$ to NPAR. NOBS is the number of observations and NPAR is the number of parameters. The diagnostic values in Jacobean matrix represent the importance of parameters. The lower sensitivity index values indicate that those parameters can be changed arbitrarily without significantly impacting the match between modeled and observed values. Therefore, it is important to address the composite sensitivity over each column for all observations. These sensitivities can also be scaled up by multiplying them with the parameter values.

The increased temperature and redistributed precipitation along with the corresponding modeled WFPS are shown in Fig. 2. The altered climate data (increased temperature and redistribution of precipitation) created summer drought characterized by WFPS lower than 60% and temperatures higher than 20 °C for most of the time. On the other hand, spring and autumn became wetter due to additional precipitation from the dry period (May to Sep). The algorithmic calibration improved the model performance as was expected (Figs. 2 and 3). However, WFPS showed closer agreement with observed data compared to $N_2O$ fluxes as shown in the scatter plot of Fig. 2. In general modeled $N_2O$ flux and WFPS matched reasonably well with measured data but on certain days were inclined to over or under estimate measured values in calibration period. The N application events produced $N_2O$ peaks in observed data. However, there is one $N_2O$ peak on day 60 which most likely occurred by N hot spot produced by a suitable temperature and rain event. The temporal variation of $N_2O$ fluxes and WFPS (measured

**Table 1**
Starting values, lower values, upper values, optimized parameter values and sensitivity values used in the calibration.

| Parameters | Starting value | Lower value | Upper value | Optimized value | Sensitivity |
|---|---|---|---|---|---|
| *rcestr(1)* | 100.00 | 50.00 | 300.00 | 98.81 | **3.12** |
| *nit_amnt* | 0.20 | 0.01 | 1.00 | 0.15 | **2.48** |
| *fleach(3)* | 0.30 | 0.20 | 0.90 | 0.22 | **2.45** |
| *epnfs(2)* | 0.01 | 0.001 | 0.10 | 0.01 | **2.22** |
| *epnfa(2)* | 0.02 | 0.002 | 0.50 | 0.03 | **1.73** |
| *water_temp* | 0.02 | 0.01 | 0.08 | 0.04 | **1.70** |
| *damr(1_1)* | 0.01 | 0.001 | 0.10 | 0.01 | **1.63** |
| *basef* | 0.20 | 0.10 | 0.90 | 0.35 | **1.55** |
| *teff(3)* | 15.00 | 10.00 | 40.00 | 12.98 | **1.53** |
| *varat12(1_1)* | 10.00 | 5.00 | 30.00 | 6.57 | **1.26** |
| *damrmn(1)* | 10.00 | 5.00 | 30.00 | 7.11 | **1.22** |
| *epnfs(1)* | 20.00 | 10.0 | 40.00 | 16.41 | **1.16** |
| *damr(2_1)* | 0.02 | 0.002 | 0.30 | 0.02 | **0.96** |
| *varat12(2_1)* | 8.00 | 4.00 | 15.00 | 6.50 | **0.91** |
| *nitrified_n* | 0.60 | 0.01 | 1.00 | 0.78 | **0.79** |
| *fleach(2)* | 0.20 | 0.10 | 0.80 | 0.17 | **0.78** |
| *peftxa* | 0.20 | 0.10 | 0.70 | 0.20 | **0.76** |
| *teff(1)* | 10.00 | 5.00 | 15.00 | 15.0 | **0.75** |
| *teff(4)* | 0.02 | 0.01 | 0.04 | 0.02 | **0.72** |
| *teff(2)* | 5.00 | 2.00 | 20.00 | 3.50 | **0.55** |
| *pabres* | 0.20 | 0.10 | 0.50 | 0.18 | **0.51** |
| *ppdf(2)* | 35 | 30 | 45 | 30 | **0.42** |
| *epnfa(1)* | 0.05 | 0.02 | 0.5 | 0.06 | **0.41** |
| *dec5(2)* | 0.30 | 0.10 | 0.80 | 0.17 | **0.40** |
| *dec1(2)* | 3.00 | 2.00 | 8.00 | 2.31 | **0.34** |
| *rces3(1)* | 4.00 | 2.00 | 10.00 | 2.75 | **0.32** |
| *varat11(1_1)* | 10.00 | 5.00 | 30.00 | 16.57 | **0.30** |
| *aneref(3)* | 0.50 | 0.20 | 2.000 | 0.51 | **0.21** |
| *dec1(1)* | 2.0 | 0.5 | 5.0 | 1.54 | **0.21** |
| *dec3(2)* | 5.0 | 3.0 | 15.0 | 12.55 | **0.20** |
| *dec2(2)* | 10.0 | 5.0 | 25.0 | 8.33 | **0.19** |
| *ppdf(1)* | 20.0 | 10.0 | 50.0 | 23.40 | **0.13** |
| *dec2(1)* | 5.0 | 3.0 | 15.0 | 12.60 | **0.11** |
| *aneref(2)* | 2.0 | 1.0 | 5.0 | 2.0 | **0.11** |
| *dec(4)* | 0.003 | 0.002 | 0.03 | 0.002 | **0.10** |
| *prdx(1)* | 0.6 | 0.1 | 2.0 | 0.65 | **0.09** |
| *drain* | 0.30 | 0.10 | 1.0 | 1.0 | **0.08** |
| *varat11(2_1)* | 8.0 | 4.0 | 15.0 | 6.50 | **0.08** |
| *fligni(1_1)* | 0.08 | 0.05 | 0.20 | 0.19 | **0.06** |
| *dec3(1)* | 4.0 | 2.0 | 8.0 | 7.28 | **0.05** |
| *rces2(2_1)* | 10.0 | 5.0 | 20.0 | 9.51 | **0.02** |
| *ddbase* | 900.0 | 800.0 | 1200.0 | 1154.01 | **0.01** |
| *fswcinit* | 0.20 | 0.10 | 0.90 | 0.72 | **0.01** |

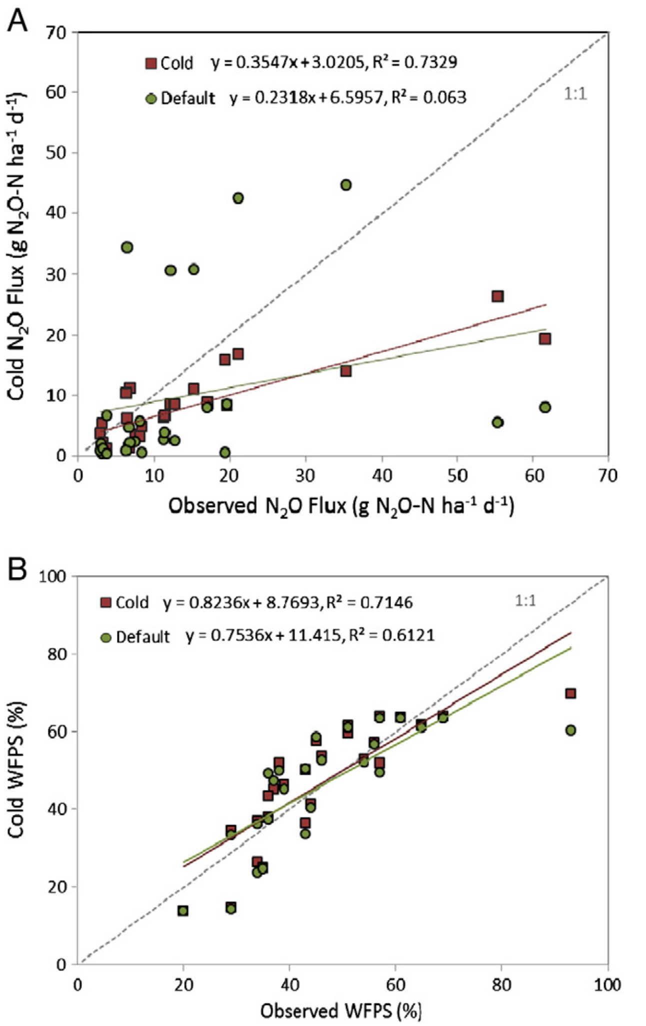


**Fig. 2.** (A) Scatter plot between observed and simulated N2O fluxes obtained from calibration runs and (B) scatter plot between observed and simulated water filled pore space (WFPS) obtained from calibrated runs. SWSR stands for the sum of weighted squared residuals observed between observed and simulated results.

and modeled) over the calibration period is shown in Fig. 3. The default simulation showed large differences between measured and modeled $N_2O$ fluxes (Fig. 3A). However, the model was not fully able to capture high $N_2O$ peaks in both the default and cold simulations. For WFPS the cold simulation results are much closer to observed data compared to default simulation (Fig. 3D). WFPS is considered a good predictor of GHG production depending on the most favorable conditions. For example $N_2O$ fluxes have been reported maximum between 60–80% WFPS values (Rafique et al., 2011a). After calibration the sum of weighted squared residual difference improved by 223% (decreased from 1635 to 505) for $N_2O$ fluxes and 22% (decreased from 623 to 507) for WFPS. Similarly, the coefficient of determination increased from 0.063 to 0.73 for $N_2O$ fluxes and 0.65 to 0.71 for WFPS.

### 3.2. GHG fluxes

#### 3.2.1. $N_2O$ fluxes

The daily $N_2O$ fluxes from both cold and manipulated simulation are shown in Fig. 3(A). The $N_2O$ fluxes are episodic in nature with small pulses throughout the year. The nature of $N_2O$ flux peaks are more pronounced in their magnitudes in manipulated simulations as compared to the results from cold simulation. The manipulated simulation showed higher peaks in spring which span over several days. In both simulations the $N_2O$ peaks occurred in response to rainfall events at optimum temperature for $N_2O$ production processes. The shift in the precipitation regime caused a different trend in $N_2O$ peaks on several occasions especially on days 60–80, 160–175 and 335–365. The daily $N_2O$ fluxes ranged from 0.81 to 33.04 g $N_2O$-N $ha^{-1}$ $d^{-1}$ for cold simulation, whereas for manipulated simulation it ranged from 0.79 to 24.73 g $N_2O$-N $ha^{-1}$ $d^{-1}$. The mean daily $N_2O$ fluxes from cold and manipulated simulations are 6.30 and 5.75 g $N_2O$-N $ha^{-1}$ $d^{-1}$ respectively. The higher peaks in both simulations are recorded in late spring and early summer corresponding to WFPS which is more than 50% during that period. Both cold and manipulated simulations were unable to capture the $N_2O$ peak events after fertilizer applications that were seen in observed $N_2O$ data.

The altered climate scenario (precipitation redistribution and increased air temperature) resulted in 9% (decreased from 2.31 to 2.10 kg $N_2O$-N $ha^{-1}$) lower annual $N_2O$ fluxes compared to cold simulation (Fig. 3A). This reduction is mainly contributed by the manipulated $N_2O$ fluxes produced in summer (May, Jun and Jul) which are 47% lower compared to cold results (Fig. 4A). Winter also showed 92% lower $N_2O$ fluxes in manipulated results, although the total contribution of winter $N_2O$ fluxes in annual sum is very low. Spring and autumn showed 29% (increased from 0.56 to 0.79 kg $N_2O$-N $ha^{-1}$) and 16 % (increased from 0.36 to 0.43 kg $N_2O$-N $ha^{-1}$) higher $N_2O$ fluxes respectively under altered climate scenario. In cold simulation summer is main source of cumulative $N_2O$ fluxes but in manipulated simulation spring is found to be main source of cumulative $N_2O$ fluxes.

#### 3.2.2. $CH_4$ fluxes

The daily $CH_4$ fluxes from both cold and manipulated simulations are shown in Fig. 3(B). In contrast to $N_2O$ emissions, the altered climate scenario resulted in overall increased cumulative $CH_4$ emissions compared to cold simulation. The $CH_4$ fluxes were characterised by small pulses throughout the year and relatively higher pulses in summer period for both cold and manipulated simulations. However, $CH_4$ peaks are more stable and less episodic than $N_2O$ emissions. The altered climate scenario resulted in elevated $CH_4$ peaks over spring and autumn period. Manipulated simulation showed higher intensity and frequency in $CH_4$ peaks compared to the cold results. The shift in the precipitation regime resulted in an opposite trend in $CH_4$ fluxes which is most obvious on days of 60–75, 135–170 and 355–365. The daily $CH_4$ fluxes ranged from 0.69 to 7.85 g $CH_4$ $ha^{-1}$ $d^{-1}$ for cold simulation, whereas for manipulated simulation it ranged from 0.59 to 8.01 g $CH_4$ $ha^{-1}$ $d^{-1}$. The mean daily $CH_4$ fluxes from cold and manipulated simulations are 4.42 and 4.92 g $CH_4$ $ha^{-1}$ $d^{-1}$ respectively. The altered climate scenario caused 10% higher annual sums of manipulated results compared to cold simulation. The annual sums of cold and manipulated results are 1.62 and 1.81 kg $CH_4$ $ha^{-1}$ respectively. This total increase in annual sum is contributed by all seasons and especially by summer which showed 15% (increased from 0.53 to 0.65 kg $CH_4$ $ha^{-1}$) higher $CH_4$ fluxes compared to cold simulation (Fig. 4B). The 2nd highest $CH_4$ source is spring which gave 11% (increased from 0.31 to 0.35 kg $CH_4$ $ha^{-1}$) higher fluxes in manipulated results compared to cold simulation. Similarly, autumn and winter contributed by 7% (increased from 0.45 to 0.49 kg $CH_4$ $ha^{-1}$) and 4% (increased from 0.31 to 0.32 kg $CH_4$ $ha^{-1}$) respectively. However, the total difference between $CH_4$ fluxes in winter is not big.

#### 3.2.3. $CO_2$ fluxes

The daily $CO_2$ fluxes from both cold and manipulated simulations are shown in Fig. 3(C). The $CO_2$ fluxes are characterized by small pulses throughout the year and higher pulses in spring and summer period for both cold and manipulated simulations. The $CO_2$ fluxes showed same episodic nature as the $N_2O$ peaks. The altered climate scenario (precipitation redistribution and increased temperature) resulted in decreased $CO_2$ emissions over most of the time period. The main $CO_2$ flux reduction occurred in spring and summer (~2000 g $CO_2$ $ha^{-1}$ $d^{-1}$). The manipulated simulation $CO_2$ fluxes in summer were recorded close to

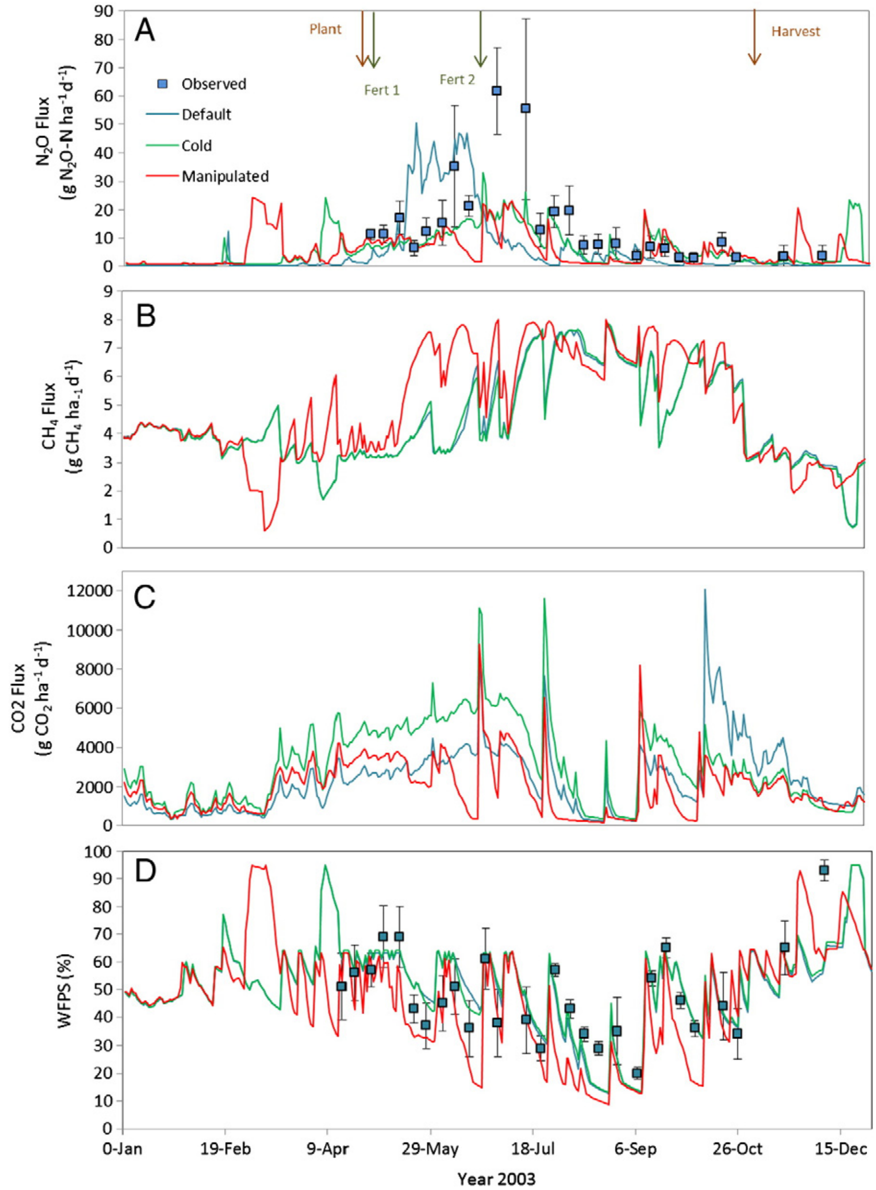


**Fig. 3.** (A) $N_2O$ flux time series from observed, default, cold and manipulated simulation results. The brown arrows show the planting and harvesting timing of crop while the green arrows show the fertilizer events, (B) CH4 flux time series obtained from default, cold and manipulated simulations, (C) CO2 flux time series obtained from default, cold and manipulated simulations and (D) water filled pore space (WFPS) time series obtained from observed, default, cold and manipulated simulations. Manipulated simulations mean the results obtained in climate scenario analysis.

zero for several days. There is not a clear pattern in the frequency of $CO_2$ flux peaks. However, $CO_2$ fluxes in the cold simulation were noticed to be more intense and higher during the whole study period. The daily $CO_2$ fluxes ranged from 295.46 to 13118.67 g $CO_2$ $ha^{-1}$ $d^{-1}$ for cold simulation, whereas for manipulated simulation it ranged from 158.44 to 9264 g $CO_2$ $ha^{-1}$ $d^{-1}$. The mean daily $CO_2$ fluxes from cold and manipulated simulations are 3098.57 and 1911.36 g $CO_2$ $ha^{-1}$ $d^{-1}$ respectively. Similarly the annual sums of cold and manipulated results are found to be 1134.08 and 699.56 kg $CO_2$ $ha^{-1}$ respectively. The altered climate scenario showed greater impact on $CO_2$ fluxes compared to $N_2O$ and $CH_4$ fluxes. The precipitation redistribution and increased air temperature resulted in 38% (decreased from 1134.08 to 699.56 kg $CO_2$ $ha^{-1}$) lower annual $CO_2$ fluxes compared to cold simulation. This reduction is contributed by all seasons and especially by summer which showed 123% (decreased from 407.99 to 182.54 kg $CO_2$ $ha^{-1}$) lower $CO_2$ fluxes compared to cold simulation (Fig. 4C). Spring and autumn showed 46% (decreased from 355.83 to 242.73 kg $CO_2$ $ha^{-1}$) and 48% (decreased from 253.79 to 171.37 kg $CO_2$ $ha^{-1}$) lower $CO_2$ fluxes respectively in manipulated simulation. Winter showed 13% (decreased from 116.45 to 102.45 kg $CO_2$ $ha^{-1}$) lower $CO_2$ fluxes in manipulated simulation which is a smaller portion in the total sum of the $CO_2$ flux.

## 4. Discussion

The biogeochemical processes that cause GHG emissions from soil are complex and involve many underlying feedback mechanisms. It is therefore difficult to develop simple empirical models that can reasonably examine GHG emissions over a range of management and climate change scenarios. By seeking to simulate underlying biogeochemical processes, models such as DAYCENT are more useful to estimate the GHG emissions from a wider range of systems including cropland. Assessing the reliability of the model is not always straight forward due to complex interactions of different model parameters. Therefore, the DAYCENT model was calibrated using advance inverse modeling software called PEST which minimizes the residual differences between modeled and observed data based on mathematical and statistical

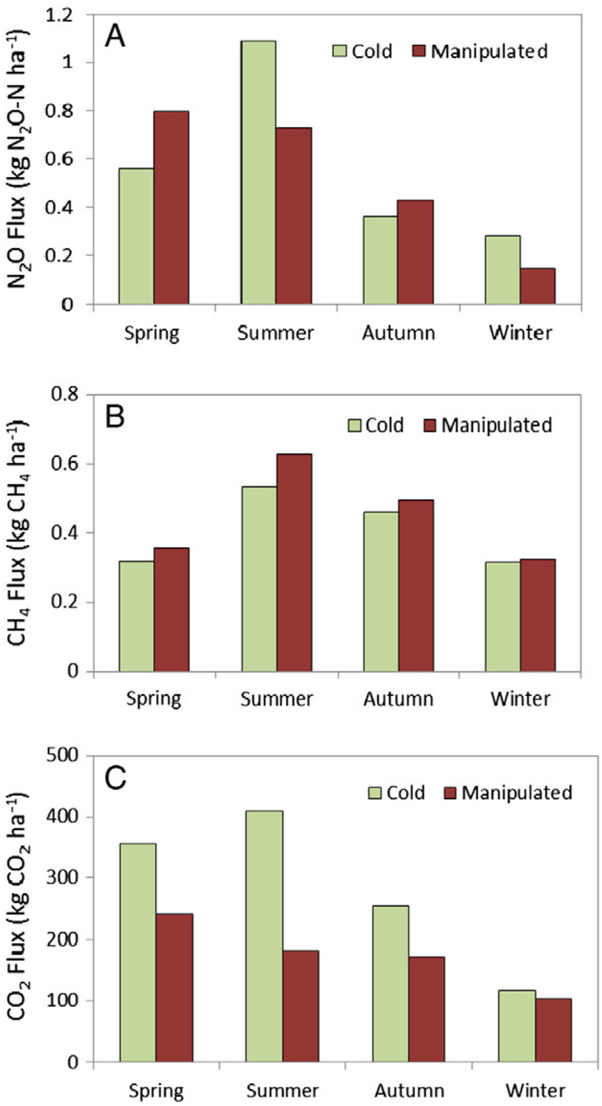


**Fig. 4.** Cumulated seasonal $N_2O$ (A), $CH_4$ (B) and $CO_2$ (C) fluxes from cold and manipulated simulations.

principles. Algorithmic calibration largely improved the model performance for this particular field study. The DAYCENT model has already been evaluated in several studies using manual calibration approaches. Compared to other DAYCENT modeling studies, our results showed better performance because of the integration of observed data into the model. For example Jarecki et al. (2008) found correlation coefficient ($r$) = 0.37 for $N_2O$ fluxes which is 129% lower than the $r$ observed in this study. Similarly, Parton et al. (2001) provided $r^2 = 0.64$ for WFPS which is 11% lower than the $r^2$ observed in this study. This is not surprising since PEST integrates observed data in DAYCENT and runs the model iteratively until minimum residual differences between observed and predicted values are achieved.

Following DAYCENT calibration the $N_2O$ flux and WFPS data generally matched measured data, but on several days it tended to over or under estimate observed values. Del Grosso et al. (2005); Jarecki et al. (2008) and Rafique et al. (2012) also reported this mismatch between daily measured and modeled data. These shortcomings of DAYCENT in predicting $N_2O$ peaks are more obvious after rain fall and fertilizer application events (Parton et al., 2001; Jarecki et al., 2008). These variations in $N_2O$ fluxes can be attributed to the natural temporal and spatial variability in N2O fluxes caused by heterogeneous soil properties and spatial distribution of N (Rafique et al., 2011a, 2012; Li et al., 2013; Kim et al., 2014) in soil. We also observed that DAYCENT did not accurately predict the soil water dynamics as was reflected in observed data. The WFPS decreased rapidly after rainfall events which might cause the large deviation in $N_2O$ peaks. Another issue can be the N fertilizer placement in the model which does not consider the spatial pattern of $NH_4^+$ and $NO_3^-$ distribution in soil (Jarecki et al., 2008). The N transformation processes such as nitrification and denitrification have also been criticized because of their over or under estimation of the rates in which N transitions to $N_2O$ fluxes. The DAYCENT model estimates denitrification for each soil layer based on $NO_3^-$ level, labile C, soil texture and water content. However, there is evidence showing that denitrifying microbial communities vary with soil depth and management practices (Del Grosso and Halvorson, 2008). The mismatch between predicted and observed $N_2O$ fluxes can also be attributed to the large uncertainties inherent in measured N2O emissions due to the complex interactions of contributing factors such as land management and soil texture (Rafique et al., 2011b). The local hot spots that occur due to N deposition (due to $NH_4^+$ and $NO_3^-$ accumulation) may cause high peaks in observed data which may not be captured in model results. Similarly, DAYCENT uses a simple land surface submodel which does not account the spatial and temporal variations of snow amounts and can cause deviation of modeled and observed WFPS data due to misinterpretation of model parameters. Effects of topography, wind, humidity, microsite heterogeneity, gas diffusion and other factors on soil water and soil temperature are likely important on daily basis but are not included in DAYCENT.

Changes in precipitation regime and temperature can potentially reduce or increase GHG emissions by altering the biological activities and land suitability. This particular process based modeling study examines the altered climate change scenario (precipitation redistribution and increased temperature) effects on GHG from cropland with NT management practices. The results obtained from both cold and manipulated simulations are noted to be comparable with other studies e.g. Ruan and Robertson (2013) and Robertson et al. (2000). We had expected that the GHG emissions and especially the $N_2O$ fluxes, would show an overall reduction in response to altered climate scenario, when the water is the most limiting factor due to a 40% reduction of precipitation (from May to September) and redistribution to wet periods (Oct, Nov, Mar and April). Extreme increases in temperature and drought events (due to lower precipitation in dry period) may have implications on soil biological activity, reducing the decomposition capability of bacteria, ultimately reducing biomass growth and soil fertility. In contrast, an increased magnitude of heavy rainfall events can cause occurrence of short periods of warm and wet conditions suitable for $N_2O$ productions. This phenomenon is noticed in spring and autumn seasons where more $N_2O$ production occurred under the increased temperature and precipitation regime scenario. However, the net $N_2O$ fluxes were lower under this scenario. This reduction can be attributed to the improved drainage under NT systems (Halvorson et al., 2010; Omonode et al., 2011).

An elevated $N_2O$ emission under NT has also been observed in other studies which was attributed to higher bulk density, more soil C and N and greater soil water content (D'Haene et al., 2008; Rochette, 2008). Six and Jastrow (2006) conducted a review study and observed higher $N_2O$ emissions in initial years following NT system, but reduced emissions after the system had been in place for 10 years or more which is in line with this study site. According to experimental evidence improved aggregate stability under NT systems can be a source of $N_2O$ emissions reduction. However, DAYCENT does not estimate the effect of changes in aggregate stability due to tillage (personal communication with Cindy Keough). Thus we cannot attribute the $N_2O$ reduction to aggregate stability in this manipulated simulation. We believe that the incorporation of aggregate stability phenomenon in DAYCENT can significantly enhance the model predictions.

In the case of $CH_4$, an increased flux in NT (Venterea et al., 2005) can occur but not always (Robertson et al., 2000). In both cases the total difference is reported to be marginal. In theory a less disturbed soil structure and improved gas diffusion in NT should enhance the $CH_4$ oxidation capacity of methanotrophic bacteria and reduce $CH_4$ emissions (Ussiri et al., 2009). In addition, there are several other studies which have shown no significant impact of NT system on $CH_4$ fluxes (Jacinthe and Lal, 2005). Therefore, the increased $CH_4$ fluxes under the altered climate scenario in this study can be attributed to increased temperature and precipitation redistribution. Increase in temperature is likely to accelerate decomposition of SOM, resulting in more $CH_4$ losses (Knorr et al., 2005). Comparatively, the effect of changes in precipitation (and hence soil moisture) on $CH_4$ from cropland is very complex. In this study the altered precipitation may result in waterlogging condition in wet periods and thus cause more $CH_4$ emissions. However, the seasonal changes in GHG pattern are very complex as they depend upon the relative influence of wetting/drying patterns. The $CH_4$ and $CO_2$ emissions are linked with each other as both are directly related with C cycle dynamics. In this study, the $CO_2$ emissions were largely reduced by increased temperature and altered precipitation regime. The major reason of this $CO_2$ emission reduction can be attributed to the NT system. According to Reicosky and Archer (2007) the total amount of $CO_2$ fluxes decreases when tillage practices do not go beyond a 10 cm depth. Ruan and Robertson (2013) reported high C sequestration and lower $CO_2$ emissions under the NT system as it slows down the SOM decomposition over longer period of time due to fewer disturbances of soil. Similarly, Patiño-Zúñiga et al. (2009) reported high OM due to higher crop residue accumulation in soil under the NT systems. Soil $CO_2$ fluxes can also be governed by temperature and soil moisture. Reichstein and Beer (2008) and Almaraz et al. (2009) showed a strong correlation of $CO_2$ fluxes with soil temperature but not with WFPS. However, WFPS is one of main controlling factor of biological activities that might affect $CO_2$ fluxes during specific times of the period. The predicted increase in C storage under drought condition in USA has been previously reported (Falloon, 2004). The uncertainties in future cropping and land use (Kumar et al., 2013) patterns make it difficult to determine the impacts of climate on cropland GHG emissions. However, the predicted changes in crop productivity can also be a source of interpretation for an increase/decrease of GHG emissions due to soil C dynamics under lower or higher yield. This study suggests that altered precipitation regime and increased temperature in the future may affect the GHG balance especially the $CO_2$ emissions under the NT systems. This altered climate scenario may also apply to other tillage regimes. However, the results can vary because of associated changes in soil properties and hence soil microbial communities. This study was purely based on model simulations which need to be compared with experimental results. We therefore recommend performing a field or laboratory experiment under increased climate warming and drought condition (precipitation distribution) to verify the mechanism of GHG emissions from soils. We also recommend performing this study for both NT and tillage regimes to see the effect of calibrated parameters.

## 5. Summary and conclusion

This study shows that the calibration using parameter estimation (PEST) software provided integrating tool for better estimates of model outputs. Sensitivity analysis provides insight into model behavior through determining the sensitive parameters. The *rcestr(1)*, *nit_amnt* and *fleach(3)* parameters showed dominant control in calibrating DAYCENT for $N_2O$ flux and WFPS. After calibration the sum of weighted squared residuals improved by 223% for $N_2O$ flux and 22% for WFPS. The increased temperature (2 °C) and altered precipitation scenario can reduce the $N_2O$ and $CO_2$ fluxes by 9% and 38% respectively, whereas the $CH_4$ emission can increase by 10%. The results of this study suggest that the drought conditions produced due to the altered climate scenario largely reduce the $N_2O$, $CH_4$ and $CO_2$ fluxes in summer season. A strong impact was observed on $CO_2$ fluxes compared to $N_2O$ and $CH_4$ emissions. The differences in frequency and intensity of GHG emissions under the altered climate scenario draw attention to this subject for potential future research. Although increased temperature and precipitation redistribution are important factors controlling GHG emissions, NT practices may also have strong impact in determining the suitable conditions required for GHG emissions. This study was based on modeling approach. We therefore suggest performing the field and laboratory experiments to further examine the GHG emissions from soil under increased temperature and drought conditions under NT systems. We also recommend applying the calibration technique in different tillage systems to see if the optimized parameters can improve the model performance.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.gloplacha.2014.05.001.

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