

## **Modeling the impacts of temperature and precipitation changes on soil CO<sub>2</sub> fluxes from a *Switchgrass* stand recently converted from cropland**

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### **Abstract**

*Switchgrass* (*Panicum virgatum* L.) is a perennial C<sub>4</sub> grass native to North America and successfully adapted to diverse environmental conditions. It offers the potential to reduce soil surface carbon dioxide (CO<sub>2</sub>) fluxes and mitigate climate change. However, information on how these CO<sub>2</sub> fluxes respond to changing climate is still lacking. In this study, CO<sub>2</sub> fluxes were monitored continuously from 2011 through 2014 using high frequency measurements from *Switchgrass* land seeded in 2008 on an experimental site that has previously used for soybean (*Glycinemax* L.) in South Dakota, USA. DAYCENT, a process-based model, was used to simulate CO<sub>2</sub> fluxes. An improved methodology CPTe [Combining Parameter estimation (PEST) with “Trial and Error” method] was used to calibrate DAYCENT. The calibrated DAYCENT model was used for simulating future CO<sub>2</sub> emissions based on different climate change scenarios. This study showed that: (i) the measured soil CO<sub>2</sub> fluxes from *Switchgrass* land were higher for 2012 which was a drought year and these fluxes when simulated using DAYCENT for long-term (2015-2070) provided a pattern of polynomial curve; (ii) the simulated CO<sub>2</sub> fluxes provided different patterns with temperature and precipitation changes in a long-

term, (iii) the future CO<sub>2</sub> fluxes from *Switchgrass* land under different changing climate scenarios were not significantly different, therefore, it can be concluded that *Switchgrass* grown for longer durations could reduce changes in CO<sub>2</sub> fluxes from soil as a result of temperature and precipitation changes to some extent.

**Keywords**

Carbon dioxide

*Switchgrass*

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## **Introduction**

*Switchgrass* is a perennial C<sub>4</sub> grass, native to North America and successfully adapted to diverse environmental conditions over large geographic regions (Lewandowski et al., 2003). It was first identified as a renewable energy source by the U.S. Department of Energy in 1985. This perennial grass can be used for livestock forage, soil stabilization, and wildlife cover. Further, *Switchgrass* can be adapted to marginal lands, and tolerates soil water deficits and low soil nutrient concentrations. Therefore, *Switchgrass* has been extensively evaluated for further development over the last two decades (Parrish and Fike, 2005; Wright, 2007). The current US average *Switchgrass* yield was projected to double or even triple by 2025 (McLaughlin et al., 2006). However, information regarding growing *Switchgrass* on marginal lands in the North Central region of USA and how does it respond to climate change when grown in a recently converted cropland is lacking.

Mitigation of carbon dioxide (CO<sub>2</sub>) emissions to the atmosphere is a key to solve the problem of global warming. It has been well documented in the literature that perennial crops emit less CO<sub>2</sub> emissions than corn (*Zea mays* L.) or soybean (Adler et al., 2007). Therefore, it can be beneficial economically and environmentally to plant *Switchgrass* on marginally yielding cropland areas over the long-term in order to mitigate the climate change impacts. However, it is very difficult to monitor climate change impacts associated with CO<sub>2</sub> fluxes. Furthermore, monitoring these CO<sub>2</sub> fluxes across the region from all possible combinations of environmental and soil conditions is very difficult (De Gryze et al., 2010). Therefore, process-based ecosystem models provide an option to simulate CO<sub>2</sub> emissions that can account for all possible permutations of management and climate in the region.

DAYCENT model (Parton et al., 1998), the daily version of the CENTURY (Parton, 1996; Parton et al., 1987), was selected in this study. It is a fully resolved ecosystem model simulating major ecosystem processes such as changes in soil organic matter, plant productivity, nutrient cycling (i.e., N, P, and S), CO<sub>2</sub> respiration, soil water, and soil temperature (De Gryze et al., 2010). However, performance of this model strongly depends on how well it is calibrated and validated for the specific environmental conditions being evaluated (De Gryze et al., 2010; Smith et al., 1997). Therefore, calibration of these models is very important in order to assess long-term

scenarios. Methods of calibrating DAYCENT used in previous studies (Chamberlain et al., 2011; Davis et al., 2010) were “trial and error” method, which is a good method but limited because it cannot obtain the best-fit values of parameters. This is a manual way of calibrating the model, as opposed to the use of statistical inverse modeling where measured data is used as input into the models to provide estimates of model parameters according to mathematical and statistical theories. The PEST (Parameter estimation) model (Doherty, 2010), a method of statistical inverse modeling, was chosen to calibrate the DAYCENT model in this study. The purpose of the PEST is to assist in data interpretation, model calibration and predictive analysis. The first statistical inverse modeling for calibrating the DAYCENT model using PEST was reported by Rafique et al. (2013). However, the method’s disadvantage is that some parameter functions and impacts in DAYCENT may be changed by PEST. For example, according to the Instruction of DAYCENT, almost parameters in fix.100 file of DAYCENT cannot be adjusted (some parameters could be adjusted with very small ranges). However, in the study by Rafique et al. (2013), some of these parameters were calibrated by PEST. This may result in biased simulations. To overcome the weaknesses of using either “*trial and error*” or *inverse modeling* method alone for model calibration, we proposed an improved methodology, i.e., combination of *trial and error* and *inverse modeling using PEST* called CPTE, which was described in our previous study (Mbonimpa et al., 2015a). In this study, the methodology has been first used for DAYCENT calibration, and to simulate climate change impacts on soil CO<sub>2</sub> fluxes.

Therefore, specific objectives of the present study were to: (i) improve the method of calibration to enhance the simulation of DAYCENT model and (ii) analyze the future long-term impacts of temperature and precipitation changes on soil surface CO<sub>2</sub> fluxes from *Switch grass* land recently converted from cropland in South Dakota.

## **1 Materials and methods**

### *1.1 Data measurements and sources*

The research site was located near Bristol (45°16' 8.274"N, 97°50'8.9694"W), South Dakota, USA. It was arranged into 12 plots measuring 21.3 m wide and 365.8 m long and comprised of three landscape positions: shoulder, backslope and footslope. Three N treatments (low, 0 kg N/ha; medium, 56 kg N/ha; and high, 112 kg N/ha) were applied annually during spring beginning in 2009. *Switchgrass* was planted on May 17, 2008 to a land previously used for

soybean production. A detailed description of the study site can be found in Mbonimpa et al. (2015b).

In this study, soil surface CO<sub>2</sub> fluxes were measured using a LI-8100 instrument (Automated Soil CO<sub>2</sub> Flux System) from plot number 103 which received the high N fertilizer rate and was located at the shoulder position. Soil CO<sub>2</sub> fluxes were monitored at every 2-hr interval for four years (2011, May 6 to November 1; 2012, April 4 to November 1; 2013, May 20 to November 13; and 2014, May 6 to October 26). The measured CO<sub>2</sub> flux data were converted to daily average values which include a total of 736 daily values, in which 85 were removed because the LI-8100 instrumentation misread and/or there were sudden and large unexplainable changes. Soil temperature and volumetric soil moisture content at 5-cm depth were measured with the soil temperature and moisture probes included with the LI-8100.

The daily maximum and minimum air temperature data for 2011 to 2013 were measured using temperature sensor connecting to the LI-8100 instrumentation at the research site. The precipitation data for 2011 through 2013 was measured by *Observation Point* which was 3.2 kilometers away from the study site. The daily maximum and minimum air temperature and precipitation from 1956 to 2010 and 2014 were retrieved from the nearest weather station in Webster, SD (25 kilometers), in which precipitation from 2001 to 2010 and 2014 were retrieved from the nearest weather station in Bristol, SD (10 kilometers). The soil bulk density and pH data were 1.37 Mg/m<sup>3</sup> and 8.09, respectively. The particle size distribution was 225 g/kg clay, 377 g/kg silt, and 398 g/kg sand.

### ***1.2 Model performance evaluation and statistical analysis***

The model performance was evaluated with five widely used quantitative criteria (Dai et al., 2014; Moriasi et al., 2007) that include the coefficient of determination ( $R^2$ , squared correlation coefficient), model performance efficiency (ME) (Nash and Sutcliffe, 1970), percent bias (PBIAS) (Gupta et al., 1999), and the RMSE and RSR [the ratio of the root mean squared error (RMSE) to SD (standard deviation of measured data)] (Singh et al., 2004). The  $R^2$  is the most important criteria to compare default simulation with that of calibrated simulation or validated simulation, and its acceptable range is  $> 0.50$  (Santhi et al., 2001). The ME is the key variable used to evaluate the model performance. If  $ME > 0.50$ , the performance is acceptable prediction. If the ME is greater than 0.65 and less than 0.75, the performance is good. If  $ME > 0.75$ , the

model performance is very good (Moriassi et al., 2007). The third important criterion is RMSE-observations standard deviation ratio (RSR). It is calculated as the ratio of the RMSE (root mean square error) and standard deviation of measured data (Singh et al., 2004). Its range of satisfactory rating values is less than 0.70 (Moriassi et al., 2007). For the PBIAS, if its absolute value is less than 25% and greater than 15%, the performance is satisfactory, and  $10\% < |\text{PBIAS}| < 15\%$  for good performance and  $|\text{PBIAS}| < 10\%$  for very good (Moriassi et al., 2007). The lower the absolute value of PBIAS, the better the performance. Further, paired simulated soil CO<sub>2</sub> fluxes between different climate scenarios were compared using the Parallel-line method because these data were time correlated values as well as each pair values were not independent. The 0.05 of significance level of the statistical hypothesis test was used. The distributions of the datasets were tested for normality using Kolmogorov-Smirnov test. The data analyses were performed using SAS 9.3 (SAS, 2012).

### ***1.3 DAYCENT model calibration and validation***

The DAYCENT model stand-alone version DailyDayCent 08/17/2014 was used for simulating soil surface CO<sub>2</sub> fluxes in this study. The model inputs include daily precipitation and maximum and minimum temperature, soil texture, bulk density, pH, and historical land use and field and crop management. In this study, “*trial and error*” method was first used to calibrate DAYCENT model. In the DAYCENT model, there are 87 parameters that can be adjusted for simulating CO<sub>2</sub>, and for this study, a total of 29 from 87 were selected based on previous literature and recommendation from model developers. The parameters values were reset on the basis of the available information for the experimental site. Then, the model was calibrated manually by adjusting values of the important parameters until the adjusted parameters improve the simulations of CO<sub>2</sub> fluxes. Through comparing the predicted CO<sub>2</sub> fluxes with those of measured values, the  $R^2$  of 0.46, ME of 0.27, RSR of 0.85, and PBIAS of -18.02% was obtained. These values were out of their acceptable ranges. Therefore, PEST model was used to calibrate further the manually calibrated DAYCENT model (called “PEST calibrated model”). Combined PEST and DAYCENT models (called “PEST calibration” or “PEST calibrated model”) were run for calibration using the most sensitive parameters ( $n = 44$ ) and measured CO<sub>2</sub> flux data from 2011 to 2013. The calibrated modeled CO<sub>2</sub> fluxes (“PEST-MOD”) were extracted from the outputs of the PEST calibrated model, and then PEST-MOD vs. measured CO<sub>2</sub> fluxes (“MEAS”) were

compared based on four statistical criteria which showed an improved calibration and prediction of CO<sub>2</sub> fluxes.

Validation of the calibrated DAYCENT was performed using (i) measured CO<sub>2</sub> fluxes in 2014, (ii) measured *Switchgrass* yields from 2009 to 2011, which were used to check the net primary productivity (NPP) that the model is predicting for this study site. It is noted that if the NPP for the site is not correct, then none of the other model outputs can be expected to be representative of the conditions at the site (Parton et al., 1998), and (iii) soil temperature and soil moisture data measured from 2011 to 2013.

#### ***1.4 Simulating and analyzing future soil surface CO<sub>2</sub> fluxes***

The PEST calibrated DAYCENT model was used to simulate CO<sub>2</sub> fluxes for long-term duration (2015 to 2070) based on future climate change scenarios, and then these simulated CO<sub>2</sub> fluxes were compared using Parallel-line method and Line charts. The future climate scenarios were created based on the method of incremental scenarios development (McCarthy, 2001). Each includes three variables: daily minimum ( $T_{\min}$  (°C)) and maximum temperature ( $T_{\max}$  (°C)) and precipitation (*Prcp* (cm)) from 2015 to 2070 based on the format of input for the DAYCENT model. The historic weather data from 1959 to 2014 were used for the observed time series to create the climate change scenarios. Based on the distribution of the observed time series (**Fig. S1A**), the maximum temperature followed a slightly decreased trend from 1959 to 2014 (**Fig. S1A**), which was stationary over time. Therefore, the maximum temperature for all scenarios was expected to increase by 0.5°C from 2015 to 2070 (total 56 years). The average increase of manual maximum temperature is 0.5/56°C. Then,  $T_{\max}$  in 2015 =  $T_{\max}$  in 1959 + 1×0.5/56°C,  $T_{\max}$  in 2016 =  $T_{\max}$  in 1960 + 2×0.5/56°C,  $T_{\max}$  in 2017 =  $T_{\max}$  in 1961 + 3×0.5/56°C, ... ,  $T_{\max}$  in 2070 =  $T_{\max}$  in 2014 + 56×0.5/56°C. For the minimum temperature, there was an increase of 2.38°C from 1959 to 2014 (**Fig. S1A**), which is non-stationary over time, therefore, the future minimum temperature for the 2015 to 2070 period could be possibly different increased trend as compared to that of 2015 to 2070 period. The increase range was expected 1°C through 3°C based on the fact of increase of 2.38°C from 1959 to 2014 and the range reported by IPCC which suggested increase in temperature roughly between 0.4°C and 2.6°C by 2060 relative to 1990 (IPCC, 2007). Within the range of 1 through 3°C, we set ten scenarios that include the minimum temperature values were increased by 1°C, 1.25°C, 1.5°C, 1.75°C, 2°C, 2.25°C, 2.38°C, 2.5°C, 2.75°C, and 3

°C from 2015 to 2070. Therefore, the magnitude of the future minimum temperatures of ten scenarios are  $2.38^{\circ}\text{C} + \text{ten different increases from 2015 to 2070} + \text{the observed } T_{\min} \text{ from 1959 to 2014, respectively}$ . For example, for the scenario 5, its minimum temperature is increased by  $2^{\circ}\text{C}$  from 2015 to 2070, its daily minimum temperature in 2015 =  $2.38^{\circ}\text{C} + T_{\min} \text{ in 1959} - 1 \times (2.38 - 2^{\circ}\text{C})/56$ , the daily  $T_{\min}$  in 2016 =  $2.38^{\circ}\text{C} + T_{\min} \text{ in 1960} - 2 \times (2.38 - 2^{\circ}\text{C})/56$ , the daily  $T_{\min}$  in 2017 =  $2.38^{\circ}\text{C} + T_{\min} \text{ in 1961} - 3 \times (2.38 - 2^{\circ}\text{C})/56$ , ... , the daily  $T_{\min}$  in 2070 =  $2.38^{\circ}\text{C} + T_{\min} \text{ in 2014} - 56 \times (2.38 - 2^{\circ}\text{C})/56$ . Based on the same algorithm,  $T_{\min}$  in other nine scenarios were calculated. Thus, the ten scenarios of temperature changes were created while *Prcp* was kept the constant. They were named as x1, x2, ..., x10, in which the x7 is corresponding to  $+ 2.38^{\circ}\text{C}$  (the amount of increase of observed minimum temperature from 1959 to 2014) and was regarded as Temperature Business As Usual (T-BAU).

The 13 scenarios of precipitation change were also created. Changes in precipitation from y1 to y13 are corresponding to -30%, -25%, -20%, -15%, -10%, -5%, 0, +5%, +10%, +15%, +20%, +25%, and +30% of the precipitation measured for 1959 to 2014. The frequencies of precipitation for future climate scenarios were kept same to that of 1959 to 2014. However, the range is based on that reported by IPCC's projected precipitation to be approximately between -30% to 30% across the globe by 2090 relative to 1990 (IPCC, 2007). The y7 is the scenario with 0% of precipitation and was regarded as Precipitation Business As Usual (P-BAU).

## 2 Results

### 2.1 Measured CO<sub>2</sub> fluxes and DAYCENT calibration and validation

Soil surface CO<sub>2</sub> fluxes from *Switchgrass* land varied seasonally and yearly (**Fig. 1A**). The higher fluxes were observed in the summer of 2012. The CO<sub>2</sub> data monitored from 2011 through 2013 were used for DAYCENT model calibration to develop the DAYCENT model, and the data from 2014 were used for validation. The most sensitive parameters in DAYCENT model were identified based on the scaled sensitivity values from PEST output. Out of 87 parameters, 44 were identified to be the most sensitive to simulate soil CO<sub>2</sub> fluxes. These parameters were ranked in descending order based on the scaled sensitivity values presented in Supplementary data of **Table 1** (i.e. **Table S1** in Supplementary data in Appendix A). The parameters *prbmn(1\_1)*, *epnfs(2)*, *sfavail(1)*, *biomax*, and *pramn(1\_1)* in the DAYCENT model were



observed to be the most sensitive. The *prbmn* (1\_1) is the intercept parameter for computing minimum C/N ratio for below ground matter as a linear function of annual precipitation. *Epnfs* (2) is intercept value for determining the effect of annual evapotranspiration non-symbiotic soil N fixation. *Sfavail* (1) is species specific fraction of N available to grass/crop. *Biomax* is biomass level above which the minimum and maximum C/E ratios of the new shoot increments equal *pramn* (\*, 2) and *pramx* (\*,2) respectively. *Pramn* (1\_1) is minimum C/N ratio with zero biomass. Other 39 parameters were described in **Table S1**. Then values of the 44 parameters were adjusted for DAYCENT calibration until the adjusted parameters improve the simulations of CO<sub>2</sub> fluxes.

Data in **Fig. 1A** showed that the simulated CO<sub>2</sub> fluxes using the manual and DAYCENT-PEST calibration were observed similar trends with those of the measured fluxes. The data reported in **Fig. 1A** showed an agreement between modeled and measured soil CO<sub>2</sub> fluxes except for few unaligned peaks. The PEST calibrated DAYCENT (DAYCENT-PEST) provided the best prediction for CO<sub>2</sub> fluxes compared to manual calibration of DAYCENT. Data in **Table 1** showed the evaluation criteria of model performance for calibration and validation periods for modeling CO<sub>2</sub> fluxes. The coefficient of determination ( $R^2$ ) value of 0.65 of the PEST calibrated DAYCENT model indicated that there was a strong linear relationship between the PEST calibrated and measured CO<sub>2</sub> fluxes, whereas,  $R^2$  of the manual calibrated model was 0.46 (**Table 1**). The percent bias (PBIAS) value of 10.28% was good for the PEST calibrated model, whereas, it was -18.02% for the manual model. Both the  $R^2$  and the PBIAS values of the PEST calibrated DAYCENT model indicated that there was not only a strong linear relationship but there was also a very close magnitude between the DAYCENT-PEST calibrated model and measured CO<sub>2</sub> fluxes. Also, modeling efficiency (ME) of 0.56 of PEST calibrated model was in the acceptable range, whereas the ME value of 0.27 of the manual model was out of the range. Further, the RSR (ratio of RMSE to standard deviation (SD) of measured CO<sub>2</sub> fluxes) value of 0.66 for the PEST calibrated model was reasonably good for the model performance, whereas, the manually calibrated model had a RSR value of 0.85, which was out of the range of satisfactory values (< 0.70). These results indicated that our final results of calibration of DAYCENT are good.

For validation, the simulated and measured CO<sub>2</sub> fluxes had similar trends and closer magnitude (**Fig. 1B**). The  $R^2$ , ME, RSR, and PBIAS values of the PEST calibrated model vs. the

manually calibrated model for the validation period were 0.63 vs. 0.52, 0.40 vs. 0.31, 0.76 vs. 0.83, and -7.88% vs. -13.92, respectively. These values of  $R^2$  and PBIAS for DAYCENT-PEST model were within satisfactory rating values compared to those of manually calibrated model (**Table 1**). The PEST vs. manually calibrated models simulated the soil temperature reasonably well with values for  $R^2$ , ME, RSR, and PBIAS of 0.86 vs. 0.86, 0.41 vs. 0.49, 0.76 vs. 0.71, and 9.78% vs. 8.36%. These values for simulating the soil moisture were 0.62 vs. 0.60, -5.41 vs. -4.76, 2.53 vs. 2.40, and -36.09% vs. -33.81%, respectively. Results in **Fig. 2a, b** showed that the simulated soil temperature data matched closely to the measured temperature. Further, modeled soil moisture content provided similar trend with the measured soil moisture but had different magnitude. For *Switchgrass* yield validation for the PEST calibrated model vs. the manually calibrated model, simulated yields of *Switchgrass* from 2009 to 2011 closely resembled the measured yields based on their PBIAS values of -1.98% vs. 0.84%, -5.19% vs. -2.50%, and -2.81% vs. 3.72% (**Table 2**). In general, the PEST calibrated DAYCENT model provided more satisfactory validation based on the above results, and hence was used for all the long-term climate scenarios.

### **2.2 $CO_2$ fluxes forecasts using BAU weather data**

The PEST calibrated DAYCENT model along with the BAU weather data was used to simulate soil  $CO_2$  from 2011 to 2070. The simulated annual  $CO_2$  fluxes from *Switchgrass* land provided a trend of polynomial curve from 2015 to 2070 (**Fig. 3a**). The curve function is:  $y = -0.0064x^3 + 0.4709x^2 - 2.9065x + 422.21$ , where  $y$  is the annual  $CO_2$  fluxes,  $x$  is year from 2015 to 2070. The simulated annual average value of  $CO_2$  fluxes from 2015 to 2070 is 554.84 ( $g/(m^2 \cdot year)$ ) with standard deviation of 103.68 and 95% confidence interval [527.07, 582.61].

### **2.3 Simulating the impacts of changing temperature scenarios on $CO_2$ fluxes**

The PEST calibrated DAYCENT model was used to simulate yearly  $CO_2$  fluxes from 2011 to 2070 based on different temperature scenarios, and then these fluxes were compared with the simulated  $CO_2$  fluxes using BAU (Note: The calculations of BAU weather data were described in the materials and methods section) (**Table S2**). Soil  $CO_2$  fluxes were not significantly affected by temperature increase from 1°C to 3°C in long-term (2015-2070) (**Table 3**). However, the annual means of simulated  $CO_2$  fluxes provided a trend of slightly linear increase with the minimum temperature increases from 1°C to 3°C (**Table 3** and **Fig. 4**).

The CO<sub>2</sub> fluxes under wet, dry and BAU were provided a trend of polynomial curves (**Fig. 3b**). The magnitude of fluxes under these three scenarios was narrower from 2015 to 2048. However, the trend and magnitude of CO<sub>2</sub> fluxes for the dry condition was different from those of wet and BAU beyond 2049. These fluctuations were wider under dry conditions than that under P-BAU and wet conditions. In contrast, CO<sub>2</sub> fluxes had a similar trend with those of BAU but the magnitude of fluxes was lower (**Fig. 3b**).

**Fig. 4** shows the simulated yearly mean CO<sub>2</sub> fluxes (g/m<sup>2</sup>/year) corresponding to ten temperature scenarios under P-BAU, wet (+30% precipitation), and dry conditions (-30% precipitation). Under wet and P-BAU condition, the CO<sub>2</sub> fluxes increased slightly with the increase of temperature, whereas, these fluxes had an observable increased trend under dry condition with the increase of temperature (**Fig. 4**). The CO<sub>2</sub> fluxes under wet condition were less than those of dry conditions and P-BAU (**Fig. 4**). The soil CO<sub>2</sub> fluxes from *Switchgrass* land in January, February, March, and December were very low, whereas, these fluxes were the highest in July. The mean CO<sub>2</sub> fluxes under wet condition from May to October were less than that under P-BAU and drought conditions, which were of similar trends and magnitudes (**Fig. S2**). The trends of monthly soil CO<sub>2</sub> fluxes were of similar trends of monthly temperature and precipitation (**Fig. S2 and S4**). Further, rates of monthly soil CO<sub>2</sub> fluxes based on scenarios of temperature changes were compared under P-BAU, wet, and drought conditions (**Table S4**). Comparing to the P-BAU and dry condition during the growing season from April to November, monthly rates of CO<sub>2</sub> fluxes under wet condition were negative and the rates in June and October were the highest. However, monthly rates of CO<sub>2</sub> fluxes under drought condition had different magnitudes of these rates, and lower than that under wet and P-BAU conditions (**Table S4**).

#### ***2.4 Simulating the impacts of changing precipitation scenarios on CO<sub>2</sub> fluxes***

The precipitation increase from +20% to +30% significantly impacted CO<sub>2</sub> fluxes compared to those from P-BAU ( $P < 0.05$ ), however, precipitation changes from -30% to +15% did not impact soil CO<sub>2</sub> fluxes ( $P > 0.05$ ) (**Table 4**).

The mean CO<sub>2</sub> fluxes with 1°C increase in temperature were slightly lower than those under temperature with BAU (T-BAU) condition (**Fig. 5**). However, a precipitation increase along with a 1°C increase in temperature resulted in slightly elevated soil CO<sub>2</sub> fluxes (**Fig. 6**). Under T-BAU and +1°C condition, the CO<sub>2</sub> fluxes had similar trends with a 2-degree polynomial curve. The data also showed that with the increase in precipitation from -30% to +30%P, the CO<sub>2</sub>

fluxes increased initially with decreased precipitation, peaked at an optimal precipitation, and then decreased to the lowest point under wet condition or increased precipitation (30%P) (**Fig. 6**). For the T-BAU trend, the maximum CO<sub>2</sub> fluxes were observed with -15%P and the trend function was given by:  $y = -295.14x^2 - 78.277x + 539$ , whereas, the maximum CO<sub>2</sub> fluxes with the +1°C temperature were observed with -5%P, and the trend function was given by:  $y = -309.7x^2 - 52.764x + 531.59$  (**Fig. 6**). The soil CO<sub>2</sub> fluxes from *Switchgrass* land in January, February, March, and December were very low, whereas, these fluxes were the highest in July. The mean CO<sub>2</sub> fluxes under T-BAU from May to October were slightly greater than that under +1°C condition (**Fig. S3**). The trends of the monthly soil CO<sub>2</sub> fluxes were of similar trends of monthly temperature and precipitation (**Figs. S3 and S4**). Further, rates of monthly soil CO<sub>2</sub> fluxes based on scenarios of precipitation changes were compared under T-BAU and +1°C conditions. All of 12 monthly rates of CO<sub>2</sub> fluxes under T-BAU condition were positive, in which November has the biggest rate of 4.06% and June has the least rate of 0.39% (**Table S4**).

### 3 Discussion

Our previous study on similar site concluded that climate impacted the soil surface CO<sub>2</sub> fluxes (Mbonimpa et al., 2014). However, to assess the potential climate change impacts on these fluxes in long-term was still a researchable question. This study showed that the CO<sub>2</sub> fluxes from *Switchgrass* land provided increased trends from 2011 to 2070 using range of different climate scenarios (**Fig. 3a, b, and Fig. 5**). These trends, however, were not a linear increase with the years but rather a polynomial. The latter trend resulted from interactions of the multiple factors those were influenced by climate. The temperature and precipitation directly determine level of soil temperature and moisture, respectively, which are the most important abiotic parameters determining CO<sub>2</sub> fluxes and its underlying processes (Kutsch et al., 2009; Subke and Bahn, 2010). Further, the future 56 years forecasting of CO<sub>2</sub> fluxes were predicted with 95% confidence interval for mean based on different climate scenarios (**Table S2**). These findings can be useful in developing greenhouse gas mitigation strategies.

Results from this study also showed that annual CO<sub>2</sub> fluxes were not significantly different for all the temperature scenarios (**Table 3**). These fluxes slightly increased with the increase in temperature (**Fig. 4**). Similarly, CO<sub>2</sub> fluxes with 13 precipitation scenarios were also not significantly different except for three scenarios (+20%, +25%, and +30%P), which resulted

in lower CO<sub>2</sub> fluxes (**Table 4 and Fig. 6**). These data indicated that impacts of long-term temperature and precipitation changes on respiration of CO<sub>2</sub> under local conditions were not significant. It has been reported in various studies that perennial grassland improves soil carbon sequestration and emit less emissions from soils. This may be the cause that in long-term climate change impacts on CO<sub>2</sub> fluxes can be minimal in *Switchgrass* land. However, a further long-term research needed to support this statement.

Soil CO<sub>2</sub> fluxes under simulated drought conditions (-30%P) were exhibited wider fluctuations in the long-term (2011-2070) (**Fig. 3b**). Some studies have shown that soil moisture affects CO<sub>2</sub> fluxes by its direct influence on root and microbial activities, and indirect influences on soil physical and chemical properties (Raich and Schlesinger, 1992; Schimel and Clein, 1996). Drought conditions reduce soil respiration and wetter conditions increase CO<sub>2</sub> production (Jensen et al., 2003; Mbonimpa et al., 2015b). The heterotrophic respiration is more susceptible to drought than autotrophic respiration (Scott-Denton et al., 2006; Zhou et al., 2007). Thus, a wide range of fluctuations in CO<sub>2</sub> fluxes under drought condition were observed compared to those under P-BAU (**Fig. 3b**). Furthermore, the CO<sub>2</sub> fluxes exhibited the slopes of increased trend with increasing temperature from 1°C through 3°C. These slopes were lower under P-BAU and wet condition compared to that with dry condition (**Fig. 4**). This may be due to the fact that *Switchgrass* performs better under soil water deficits. The present study site is located under the humid continental climate which is still appropriate for *Switchgrass* to grow well even if the precipitation amount were reduced by 30% compared to the P-BAU. Furthermore, the cultivar of *Switchgrass* for the study site was developed for local conditions. The improved *Switchgrass* growth could increase the respiration of CO<sub>2</sub> with temperature under dry conditions compared to that under wet conditions. However, under wet conditions, higher water content in soils decreased air-filled porosity, increased stomatal resistance and hence decreased CO<sub>2</sub> respiration (Kirkham, 2011).

These results also indicated that when temperature is kept as constant, both dry and wet conditions could decrease CO<sub>2</sub> emissions (**Fig. 6**). Some studies have shown that there is a negative effect of elevated soil temperature on soil moisture due to increased evapotranspiration (Liu et al., 2009; Poll et al., 2013; Shaver et al., 2000). Additionally, it is not necessarily true that precipitation always increases moisture content of the soils probably because most precipitation events were unlikely to rewet the soil to a greater depth (Poll et al., 2013). The reduction in soil

moisture by soil warming was shown to reduce microbial respiration in a dry semiarid temperate steppe (Liu et al., 2009). This inconsistency between soil moisture and soil respiration is probably due to the above mentioned inability of precipitation events to rewet the dry soil to a depth of 15 cm (Poll et al., 2013), especially, at the shoulder position as is the case in our research site. Under moisture excess or waterlogged conditions, there were anaerobic conditions and suppression of CO<sub>2</sub> emissions (Liu et al., 2002). Furthermore, higher water content in soils is a condition attributed to reduced transpiration due to increased stomatal resistance (Kirkham, 2011). These conditions could result in lack of oxygen in soil organic matter, which subsequently decreases respiration. Therefore, the CO<sub>2</sub> fluxes were lower wet conditions compared to dry and BAU.

Soil surface CO<sub>2</sub> fluxes were higher with the T-BAU (+2.381°C) compared to that with +1°C condition (**Fig. 6**). This was primarily because temperature increased CO<sub>2</sub> emissions with increased soil organic matter decomposition. Further, precipitation amount contributing to the maximum CO<sub>2</sub> flux under T-BAU was lower than that under +1°C condition (**Fig. 6**). This might be explained by higher temperature values that can reduce soil moisture content through the evaporation process and increasing decomposition of organic compounds in aerobic soils. Further, the humid continental climate at the study site could result in the maximum CO<sub>2</sub> fluxes under the reduced precipitation conditions, indicating that properly managed *Switchgrass* in the present site has the potential to mitigate CO<sub>2</sub> fluxes. Data from this study showed that increased precipitation with increased temperature produced higher CO<sub>2</sub> fluxes. These findings were also supported by other researchers who reported that the main driving factors affecting belowground soil respiration were temperature, precipitation or temperature in combination with precipitation (Do, 2008). The interactions of soil temperature and moisture determine soil respiration in most ecosystems (Kanerva et al., 2007; Li et al., 2006). Regression analysis showed that soil moisture positively affected the correlation between soil temperature and soil respiration and explained 25% of the variation in Q<sub>10</sub> values (Poll et al., 2013). The increase in CO<sub>2</sub> fluxes under higher temperature condition may be explained by increased plant biomass in general and subsequent increases in C flow to the soil with increase of temperature and precipitation (Kanerva et al., 2007).

#### **4 Conclusions**

Soil surface CO<sub>2</sub> fluxes are strongly influenced by climate, however, evaluating impacts of different climate scenarios on these fluxes in long-term is difficult without modeling tools. Our previous study that included measured CO<sub>2</sub> data for 3 years showed that climate significantly impacted the CO<sub>2</sub> fluxes. Therefore, this study was conducted to assess the long-term impacts of climate on CO<sub>2</sub> fluxes from *Switchgrass* land recently converted from cropland. DAYCENT model was used for assessing the climate change scenarios. The calibration of this model was improved using a new (CPTE) methodology that combines the “trial and error” and PEST model to reduce the biasness of model predictions. The four data (CO<sub>2</sub> fluxes of 2014, *Switchgrass* yield from 2009 to 2011, and soil temperature and soil moisture from 2011 to 2013) were used for validating the model. Then the calibrated and validated DAYCENT model was used to simulate and analyze future CO<sub>2</sub> fluxes.

This study concluded that measured soil CO<sub>2</sub> fluxes were higher for 2012 which was a drought year, and these fluxes when simulated for long-term (2015-2070) provided an increased pattern of polynomial curve. Soil surface CO<sub>2</sub> fluxes from *Switchgrass* land showed an increased trend from 2011 to 2070 with a polynomial curve. The distribution patterns of temperature and precipitation were more important for soil CO<sub>2</sub> efflux seasonal dynamics. Our simulation results showed that the future CO<sub>2</sub> emissions from *Switchgrass* land in South Dakota, generally, would be insignificantly different with temperature and precipitation, therefore, *Switchgrass* grown for longer durations could reduce changes in CO<sub>2</sub> fluxes from soil as a result of temperature and precipitation changes within the ranges of the climate scenarios to some extent. However, to assess the climate change impacts based on just one parameter was not sufficient, therefore, the future work needs that include a systematical analysis of different parameters such as greenhouse gas (GHG) fluxes, soil organic carbon, total nitrogen and other crops and soils data from *Switchgrass* land.

## **Acknowledgments**

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## Appendix A. Supplementary data

Supplementary data to this article can be found online version.

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**Fig. 1 (A)** Calibration: distribution of measured and modeled values of CO<sub>2</sub> (g/m<sup>2</sup>/day) fluxes from 2010 through 2013, **(B)** validation: distribution of measured and modeled values of CO<sub>2</sub>

(g/m<sup>2</sup>/day) fluxes from 2014. MEAS, measured; PEST-MOD, calibrated modeled CO<sub>2</sub> fluxes using PEST model; and MAN-MOD, manually calibrated modeled CO<sub>2</sub> fluxes using “trial and error” method.

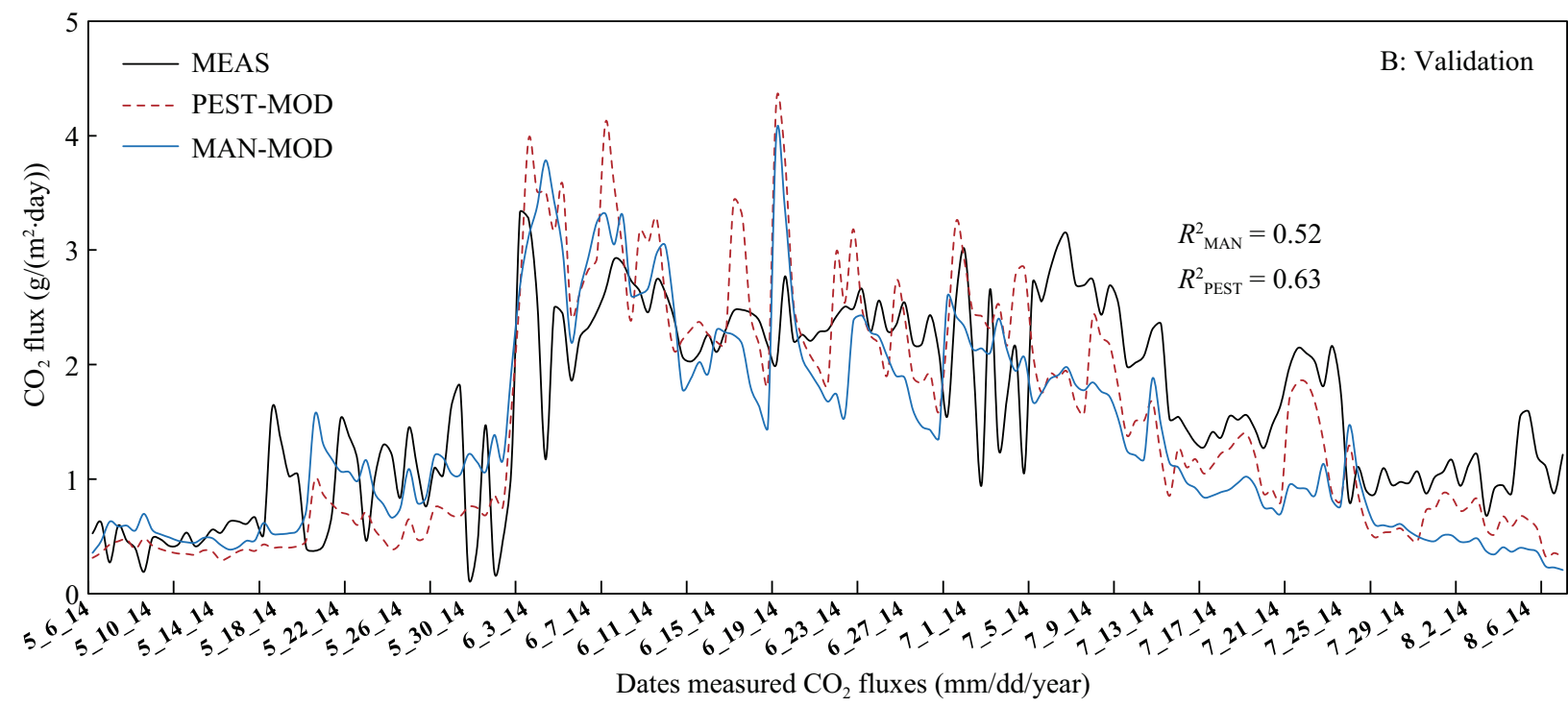
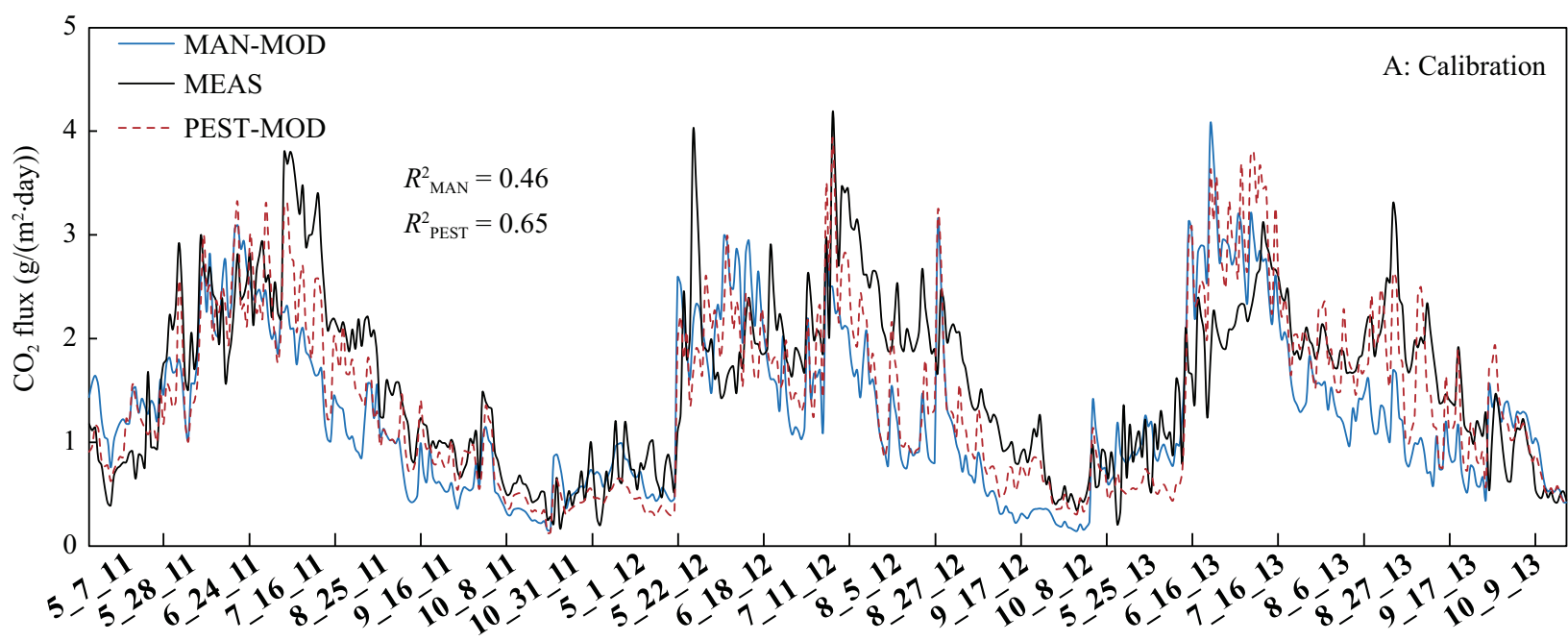
**Fig. 2** Comparison of measured and simulated soil temperature (a), and soil moisture content (b) for validation. MEAS, measured values; PEST-MOD, calibrated modeled values using PEST model; and MAN-MOD, manually calibrated modeled values using “trial and error”.

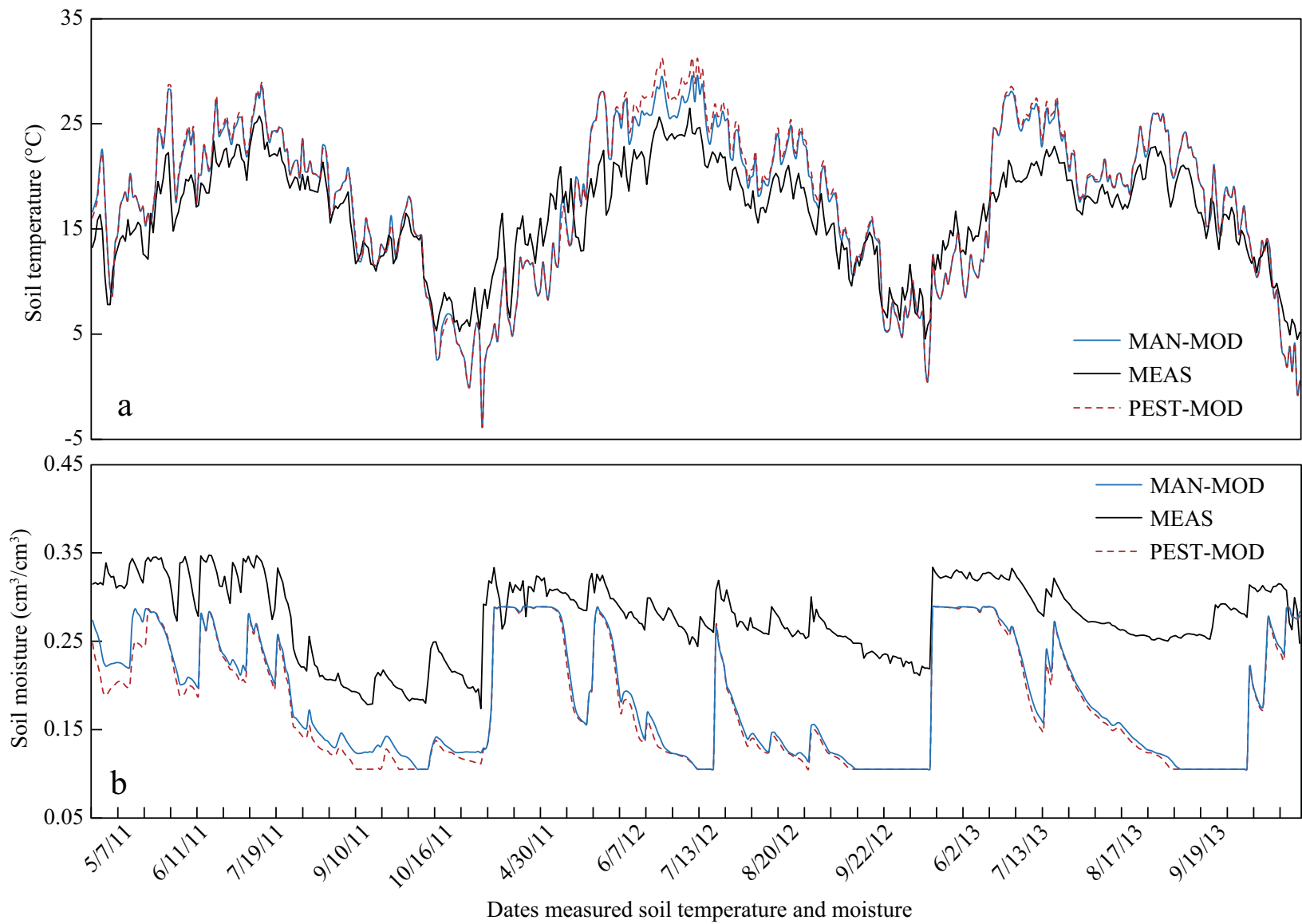
**Fig. 3** Average annual simulated CO<sub>2</sub> fluxes from 2015 to 2070 simulated using (a) the weather data of BAU and (b) temperature scenarios from 2011 to 2070 under dry, wet, and P-BAU conditions.

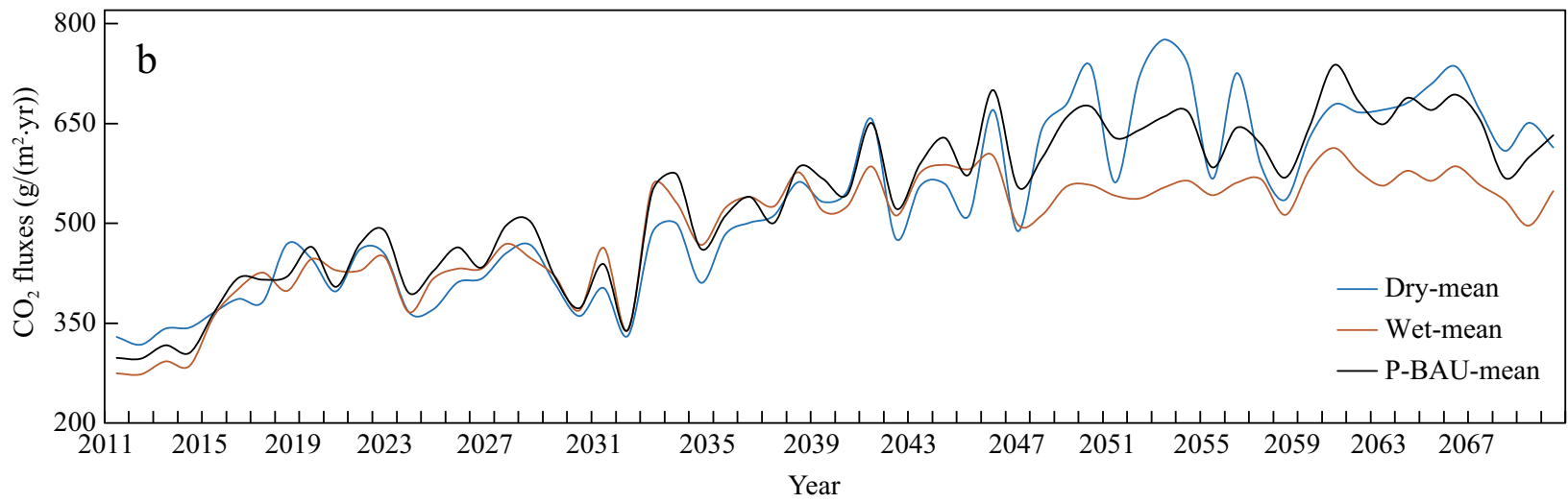
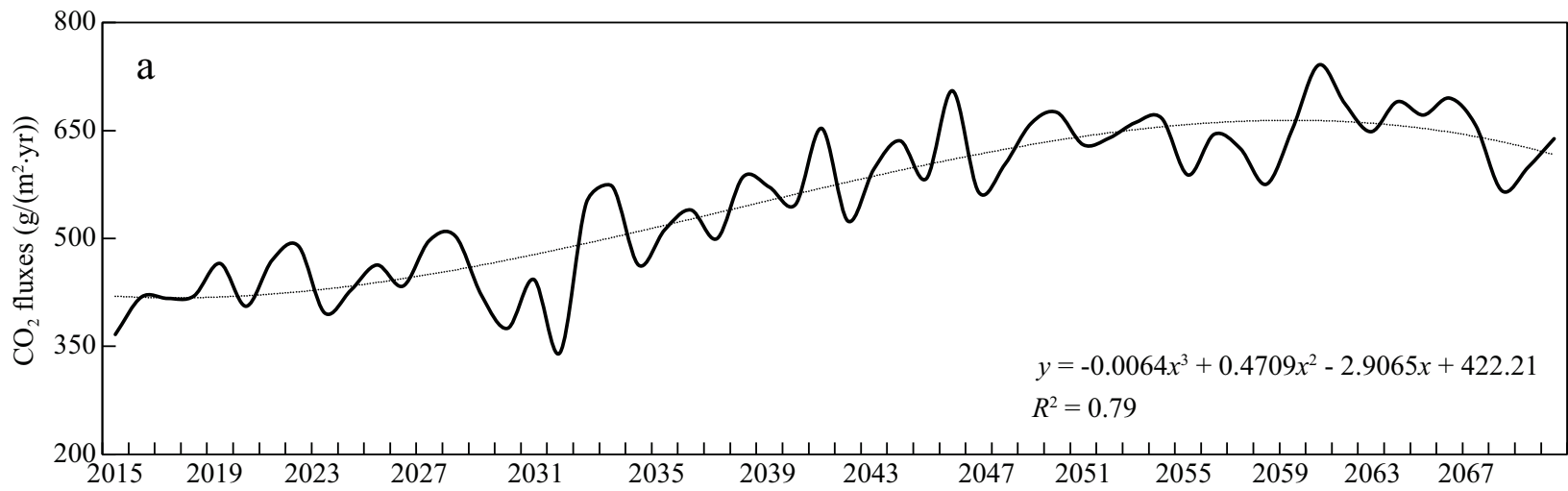
**Fig. 4** Average annual simulated CO<sub>2</sub> fluxes corresponding to temperature scenarios +1 through +3°C under dry, wet, and P-BAU conditions.

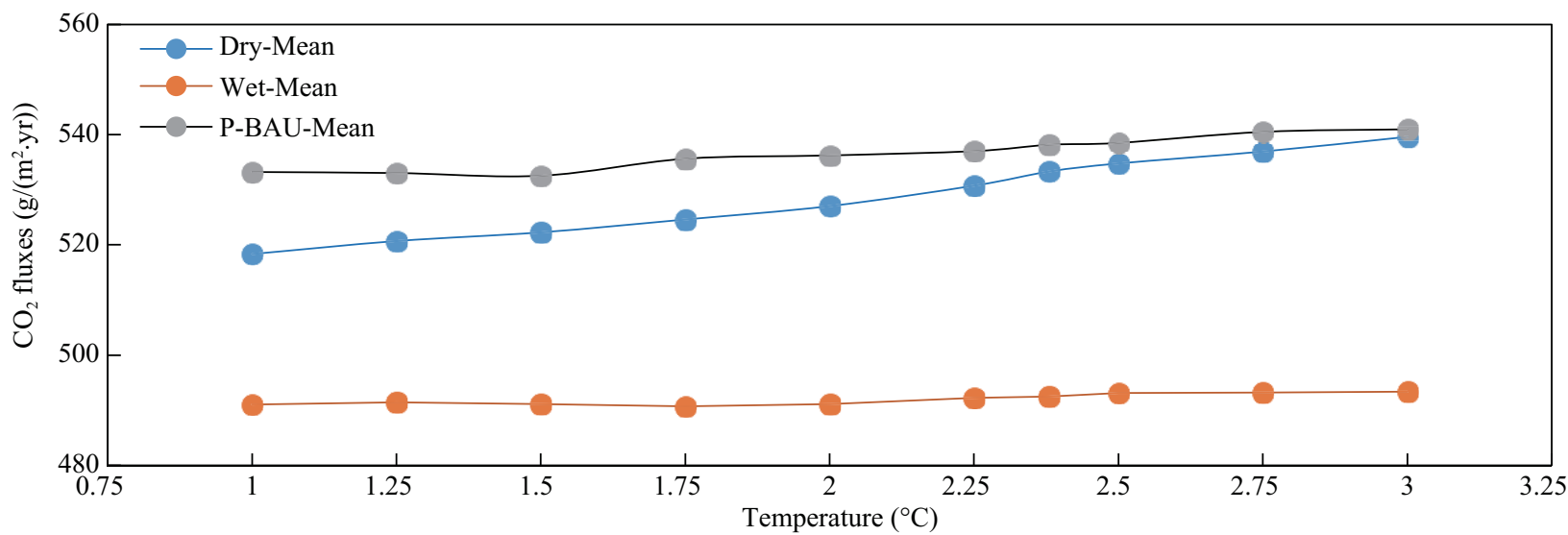
**Fig. 5** Trends of simulated average annual CO<sub>2</sub> fluxes from 2011 to 2070 based on precipitation changes from -30% to +30% under temperature of BAU (increase of 2.38°C) and increase of 1°C with years.

**Fig. 6** Trends of simulated average annual CO<sub>2</sub> fluxes from 2011 to 2070 based on precipitation changes from -30% to +30% under temperature of BAU (increase of 2.38°C) and increase of 1°C with changing precipitation.

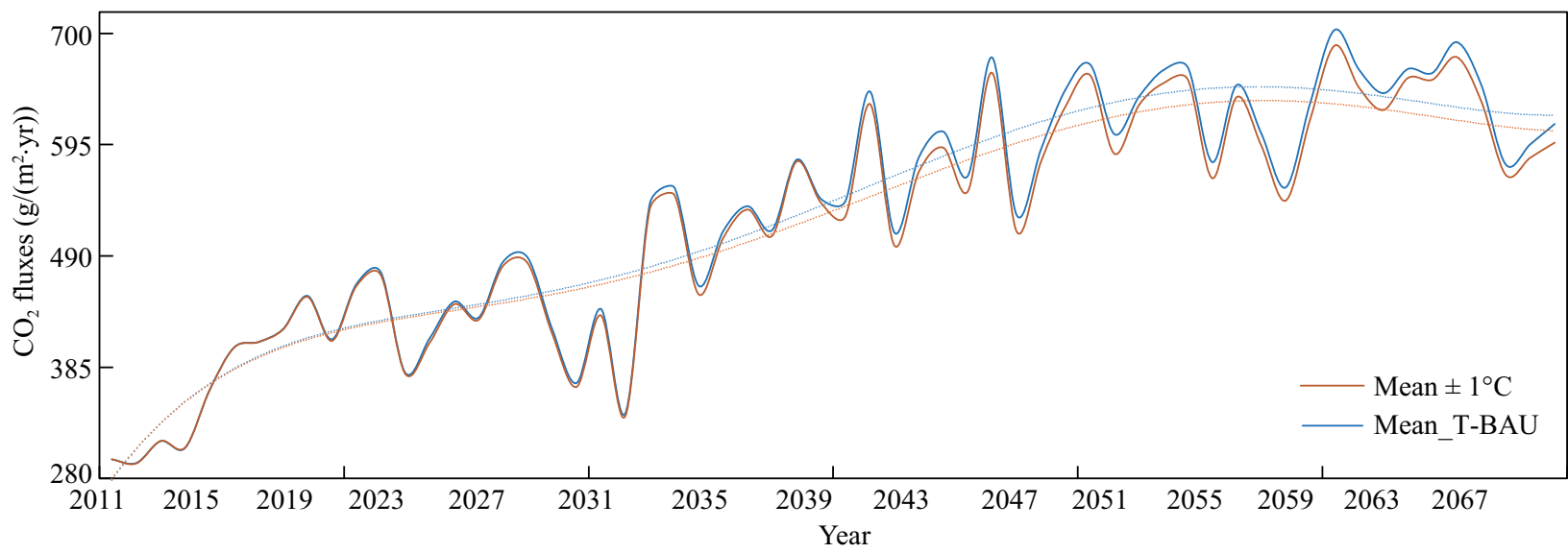


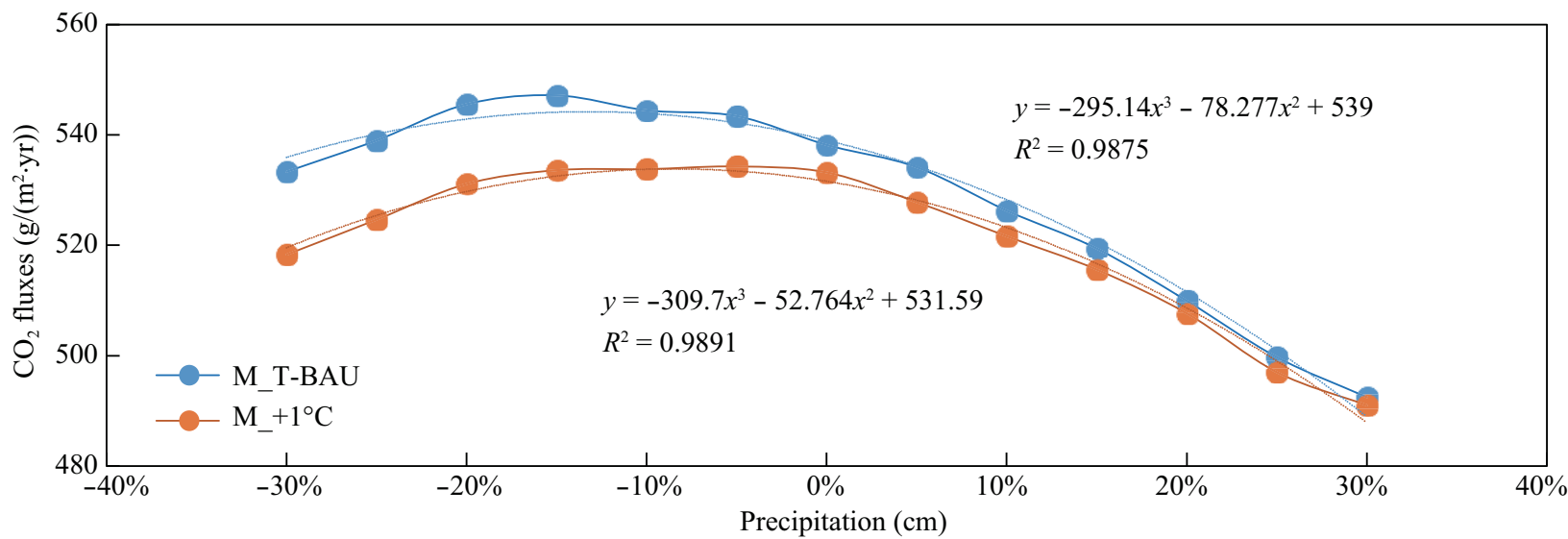












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**Table 1** Evaluation criteria for comparing soil surface CO<sub>2</sub> fluxes, soil temperature, and soil moisture between measured and modeled data using manually calibrated DAYCENT (Manual) and PEST calibrated DAYCENT (PEST) model for calibration and validation.

Evaluation Criteria <sup>†</sup>	Calibration		Validation					
	CO <sub>2</sub> (g/(m <sup>2</sup> ·day))		CO <sub>2</sub> (g/(m <sup>2</sup> ·day))		Soil temperature (°C)		Soil moisture (cm <sup>3</sup> /cm <sup>3</sup> )	
	Manual	PEST	Manual	PEST	Manual	PEST	Manual	PEST
$R^2$ ((0.5,1))	0.46	0.65	0.52	0.63	0.86	0.86	0.60	0.62
ME ((0.5, 1))	0.27	0.56	0.31	0.40	0.49	0.41	-4.76	-5.41
RSR ((0.7, 0))	0.85	0.66	0.83	0.78	0.71	0.76	2.40	2.53
PBIAS ((25%, 0))	-18.02	-10.28	-13.92	-7.88	8.36	9.78	-33.81	-36.09

<sup>†</sup> $R^2$  = coefficient of determination; ME = modeling efficiency; RSR = the ratio of the root mean squared error to standard deviation of measured data; and PBIAS = percent bias.

**Table 2** Comparison of modeled and measured *Switchgrass* yield (g/(m<sup>2</sup>·year)) for validation.

Year	Measured	DAYCENT-PEST		DAYCENT	
		Modeled	PBIAS (%)	Modeled	PBIAS (%)
2009	303.88	297.87	-1.98	300.37	0.84
2010	566.69	537.30	-5.19	523.87	-2.50
2011	545.21	529.89	-2.81	549.61	3.72

**Table 3** Statistical results of comparing simulated future soil CO<sub>2</sub> fluxes (g/(m<sup>2</sup>·year)) based on different temperature scenarios.

CO <sub>2</sub> fluxes - temperature changes					
Var <sup>[1]</sup>	Mean ± SD	L95%CI	U95%CI	p-value <sup>[2]</sup>	
x1	533.19 ± 115.33	503.40	562.98	x1/x7:0.63	-
x2	533.00 ± 115.33	503.21	562.80	x2/x7:0.62	x2/x1:0.99
x3	532.51 ± 115.26	502.74	562.29	x3/x7:0.59	x3/x2:0.96
x4	535.61 ± 117.44	505.27	565.94	x4/x7:0.81	x4/x3:0.77
x5	536.21 ± 117.16	505.94	566.47	x5/x7:0.85	x5/x4:0.95
x6	536.99 ± 117.81	506.56	567.43	x6/x7:0.91	x6/x5:0.94
x7	538.15 ± 118.28	507.60	568.71	-	x7/x6:0.91
x8	538.48 ± 118.50	507.87	569.09	x8/x7:0.97	x8/x7:0.89
x9	540.50 ± 119.34	509.67	571.33	x9/x7:0.82	x9/x8:0.85
x10	540.97 ± 119.72	510.04	571.90	x10/x7:0.79	x10/x9:0.96

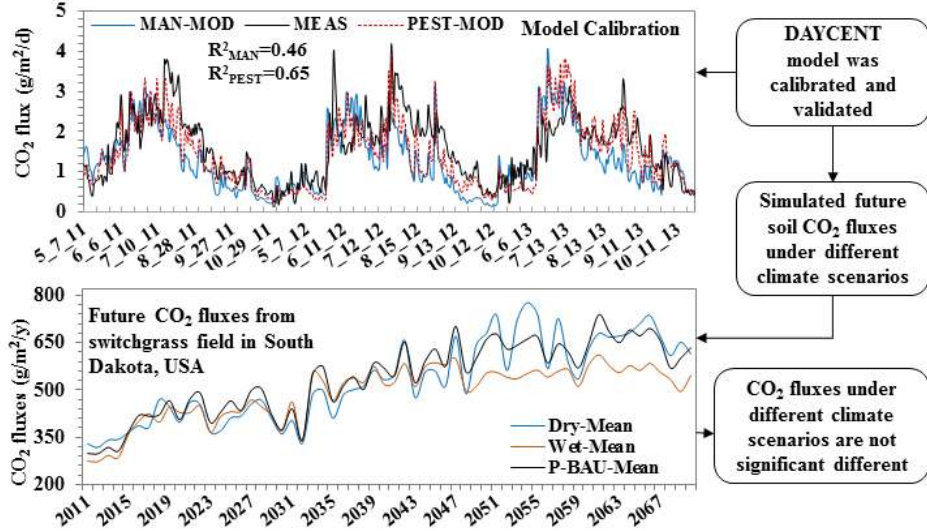
[1] x1=+1°C; x2=+1.25°C; x3=+1.5°C; x4=+1.75°C; x5=+2°C; x6=+2.25°C; x7=+2.38°C; x8=+2.5°C; x9=+2.75°C; x10=+3°C. [2] p-values were from output of Parallel line analysis.

**Table 4** Statistical results of comparing simulated future soil CO<sub>2</sub> fluxes (g/(m<sup>2</sup>·year)) based on different precipitation scenarios.

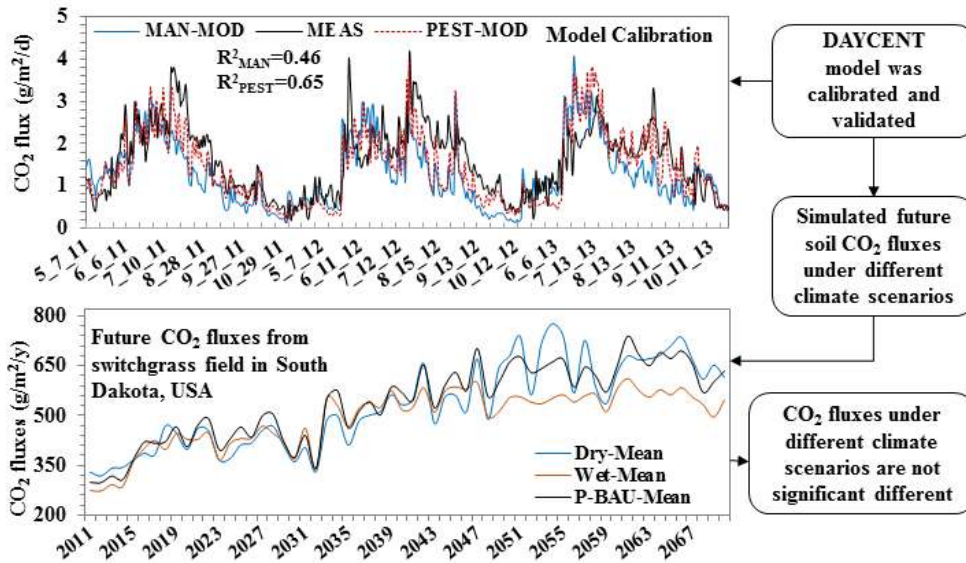
CO <sub>2</sub> fluxes - precipitation changes					
Var <sup>[1]</sup>	Mean±SD	L95%CI	U95%CI	p-value <sup>[2]</sup>	
y1	533.30 ± 133.60	498.79	567.82	y1/y7:0.53	-
y2	538.97 ± 134.66	504.18	573.75	y2/y7:0.86	y2/y1:0.65
y3	545.53 ± 139.66	509.45	581.61	y3/y7:0.78	y3/y2:0.65
y4	547.12 ± 136.34	511.90	582.34	y4/y7:0.64	y4/y3:0.85
y5	544.42 ± 130.76	510.64	578.20	y5/y7:0.75	y5/y4:0.88
y6	543.38 ± 125.84	510.87	575.88	y6/y7:0.75	y6/y5:0.99
y7	538.15 ± 118.28	507.60	568.71	-	y7/y6:0.75
y8	534.12 ± 113.73	504.74	563.50	y8/y7:0.78	y8/y7:0.78
y9	526.26 ± 106.28	498.80	553.71	y9/y7:0.4	y9/y8:0.58
y10	519.39 ± 100.53	493.42	545.36	y10/y7:0.18	y10/y9:0.62
y11	509.93 ± 96.56	484.98	534.87	y11/y7:0.039	y11/y10:0.44
y12	499.73 ± 93.36	475.61	523.85	y12/y7:0.004	y12/y11:0.40
y13	492.48 ± 89.24	469.42	515.53	y13/y7<0.001	y13/y12:0.56

[1] y1 = -30%P; y2 = -25%P; y3 = -20%P; y4 = -15%P; y5 = -10%P; y6 = -5%P; y7 = 0%P; y8 = 5%P; y9 = 10%P; y10 = 15%P; y11 = 20%P; y12 = 25%P; y13 = 30%P. [2] p-values were from output of Parallel line analysis.

- An improved methodology CPTE was used to calibrate and validate DAYCENT model.
- Switchgrass offered the potential to reduce soil CO<sub>2</sub> fluxes with climate change.
- The simulated CO<sub>2</sub> fluxes provided different patterns with temperature and precipitation changes in a long-term.



Draft 1 of the graphical abstract.



Draft 2 of the graphical abstract.

**Our suggestion:** Please use Draft 2. Please change “CO<sub>2</sub> flux (g/m<sup>2</sup>/d)” into “CO<sub>2</sub> flux (g/(m<sup>2</sup>.day))” in top figure, change “CO<sub>2</sub> fluxes (g/m<sup>2</sup>/y)” into “CO<sub>2</sub> flux (g/(m<sup>2</sup>.yr))” in bottle figure.