Predicting soils and environmental impacts associated with switchgrass for bioenergy production: a DAYCENT modeling approach

LIMING LAI1, SANDEEP KUMAR1, SOLOMON M. FOLLE2 and VANCE N. OWENS3
1Department of Agronomy, Horticulture and Plant Science, South Dakota State University, Brookings, SD 57007, USA,
2Farmers Edge, Shakopee, MN 55379, USA, 3North Central Sun Grant Center, South Dakota State University, Brookings, SD 57007, USA

Abstract

Switchgrass (Panicum virgatum L.) production has the potential to improve soils and the environment. However, little is known about the long-term future assessment of soil and environmental impacts associated with switchgrass production. In this study, soil organic carbon (SOC), soil nitrate (NO₃⁻), water-filled pore space (WFPS), carbon dioxide (CO₂) and nitrous oxide (N₂O) fluxes, and biomass yield from switchgrass field were predicted using DAYCENT models for 2016 through 2050. Measured data for model calibration and validation at this study site managed with nitrogen fertilization rates (N rates) (low, 0 kg N ha⁻¹; medium, 56 kg N ha⁻¹; and high, 112 kg N ha⁻¹) and landscape positions (shoulder and footslope) for switchgrass production were collected from the previously published studies. Modeling results showed that the N fertilization can enhance SOC and soil NO₃⁻, but increase soil N₂O and CO₂ fluxes. In this study, medium N fertilization was the optimum rate for enhancing switchgrass yield and reducing negative impact on the environment. Footslope position can be beneficial for improving SOC, NO₃⁻, and yield, but contribute higher greenhouse gas (GHG) emissions compared to those of the shoulder. An increase in temperature and decrease in precipitation (climate scenarios) may reduce soil NO₃⁻, WFPS, and N₂O flux. Switchgrass production can improve and maintain SOC and NO₃⁻, and reduce N₂O and CO₂ fluxes over the predicted years. These findings indicate that switchgrass could be a sustainable bioenergy crop on marginally yielding lands for improving soils without significant negative impacts on the environment in the long run.

Keywords: carbon dioxide flux, DAYCENT model, nitrous oxide flux, soil nitrate, soil organic carbon, switchgrass (Panicum virgatum L.)

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Introduction

Switchgrass (Panicum virgatum L.) is a perennial grass (C₄) and native to North America and can adapt to different environmental conditions due to its tolerance to soil water deficits and low soil nutrients (Lewandowski et al., 2003). In addition to the traditional uses of switchgrass for livestock forage, soil stabilization, and wildlife cover, it became a significant renewable energy source identified by the U.S. Department of Energy in 1985 (Lee et al., 2012) and was selected as a ‘model’ potential bioenergy crop in 1991 (Wright & Turhollow, 2010). Switchgrass production can help in reducing soil erosion, increasing soil organic carbon (SOC), improving water quality and wildlife habitat, and mitigating net greenhouse gas (GHG) emissions from soils (Daly et al., 2008; Blanco-Canqui, 2010). However, these results are from different studies that separately analyzed a few parameters for short term, thereby the comprehensive impacts of switchgrass production on soils and the environment are still lacking, and the sustainability feasibility of the biofuel expansion is still uncertain. Furthermore, it is estimated that there could be more than 30% of demand for biofuels by 2050 (IEA, 2011), and thereby, the bioenergy crop production could be critical for the future environmental impacts and climate change mitigation (Oliveira et al., 2017). Evaluating long-term future impacts of switchgrass production on soils, biomass yield, and GHG emissions from soils is vital for government organizations to make policy that supports switchgrass as a bioenergy feedstock.

Biogeochemical process models are useful tools for conducting the comprehensive assessment of the impacts of switchgrass production on soils and GHG emissions (Del Grosso et al., 2006; Abdalla et al., 2010) and evaluating the impacts of agricultural practices and climate change on crop growth, yield, soil and hydrological properties, and soil GHG emissions simultaneously (Olander et al., 2011). The DAYCENT model
(Parton et al., 1998), the daily version of CENTURY model (Parton et al., 1987; Parton, 1996), was selected in this study because (i) this model can simulate major ecosystem processes via different parameters (e.g., soil properties, plant productivity, and GHG fluxes etc.) with daily outputs (Parton et al., 1998) and (ii) it is currently used for the US inventory of GHG budgets (Olander et al., 2011). However, the model must be calibrated and validated using the measured data under specific environmental conditions (Smith et al., 1997; De Gryze et al., 2010). Some studies have used DAYCENT model for analyzing switchgrass sustainability. For example, Chamberlain et al. (2011) predicted a decrease in GHG emissions and nitrate runoff from soils managed under cotton (Gossypium hirsutum L.) converted to switchgrass in the Southern U.S. Hudiburg et al. (2015) estimated that replacement of corn (Zea mays, L.)–soybean (Glycine max L.) rotations would result in a net GHG emission reduction for switchgrass in the Midwest and the Eastern United States. Davis et al. (2012) reported that conversion from corn to switchgrass for biofuel production can transition the central United States from a net source to a net sink for estimated GHGs. Our previous publication using DAYCENT model predicted that switchgrass production for longer durations could diminish changes in soil surface carbon dioxide (CO$_2$) emissions based on potential future changes in temperature and precipitation in South Dakota (Lai et al., 2016). However, the information regarding the long-term comprehensive assessment of switchgrass production impacts on soil, water, and GHG emissions is still lacking.

The DAYCENT models in this study were built, calibrated, and validated based on the measured data and information from the switchgrass field established on a marginal land managed with the three nitrogen (N) fertilization rates (N rates) and the two landscape positions in South Dakota (Mbonimpa et al., 2015b). The N fertilization can significantly influence switchgrass growth and the environment. An adequate amount of N fertilization can enhance SOC accumulation, soil fertility (Bowman & Halvorson, 1998), and switchgrass biomass yield (Owens et al., 2013; Hong et al., 2014) and reduce soil nitrate (NO$_3^-$) leaching and nitrous dioxide (N$_2$O) emissions from soils (Reay et al., 2012). If excessive N fertilizer is applied, it could result in N losses such as NO$_3^-$ leaching and N$_2$O emissions (Follett, 1995; Luce et al., 2011). However, specific information about the effect of N rate on soils and the environment in switchgrass field is still lacking. Landscape position is a key factor influencing the soil properties in crop–soil systems under a hillslope scale (Guzman & Al-Kaisi, 2011; Majaliwa et al., 2015). The field-scale soil properties such as SOC, soil NO$_3^-$, soil phosphorus (P), soil bulk density ($\rho_b$), and pH under switchgrass are quite variable depending on different sites (e.g., Schmer et al., 2011). However, little is known about landscape position effects on the environment under switchgrass field. The information about the effects of N rate and landscape position on switchgrass production will be helpful for the producers to manage their fields and enhance their economic incomes. Meanwhile, fluctuations in climate can also impact the processes and factors controlling soils and the environment (Brevik, 2012). These climatic fluctuations not only impact soil water content and soil temperature but also soil mineral N and carbon (C) availability, influencing GHG emissions from soils (Alvaro-Fuentes et al., 2017). In this study, the two future climate scenarios (S2 and S4) were chosen for evaluating the climate impacts on soils and the environment associated with switchgrass production for bioenergy. This was because the S2 and S4 scenarios were generated in response to intermediate emissions scenario 2 under the Representative Concentration Pathway (RCP) 4.5 W m$^{-2}$ and high emissions scenario 4 under the RCP 8.5 W m$^{-2}$, respectively, based on Inter-governmental Panel on Climate Change (IPCC) Expert Meeting Report (2008) (Moss et al., 2008). The future emission scenario 4 would be nearly double, compared with the emission scenario 2.

The SOC, soil NO$_3^-$, water-filled pore space (WFPS), CO$_2$ and N$_2$O fluxes from soils, and switchgrass biomass yield were selected in this study for the future assessment using the DAYCENT models. Dynamics of SOC in agricultural soils can drive microbial activity and nutrient cycles, promote soil physical properties and water retention capacity, and reduce erosion (Manna et al., 2007; Dong et al., 2012). The increased SOC stock can reduce net soil surface CO$_2$ emissions, which is the primary GHG that is contributing to global warming potential, which can result in climate change (EPA, 2016). The WFPS requires only a knowledge of soil water content and soil bulk density (Linn & Doran, 1984), indicating that the WFPS is a more practical index of soil aeration that mostly determines the aerobic microbial activities (Skopp et al., 1990). The NO$_3^-$ is the major inorganic N form that can be taken up by crops. It is converted from the inorganic ammonium (NH$_4^+$) under appropriate climatic conditions through nitrification (Whalen & Sampedro, 2010). However, the excessive NO$_3^-$ in soils can leach into the underground water (Lamb et al., 2014), causing water quality problems in natural water systems (Ma et al., 2001; Madakadze et al., 2003). The extra soil NO$_3^-$ can also be converted to N gases such as N$_2$O emissions that are lost to the atmosphere through denitrification (Luce et al., 2011). The excessive N$_2$O in the atmosphere can contribute to global warming, and

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currently, it is the single most important ozone-depleting emission (Dai et al., 2014).

The objectives of this study therefore were to (i) predict the selected parameters (SOC, NO$_3$$_2$, WFPS, CO$_2$ and N$_2$O fluxes, and switchgrass biomass yield) using DAYCENT models, and (ii) evaluate the impacts of the N rate, landscape position, and climate change on these parameters, and further assess the impacts of switchgrass production on soils and the environment over time.

Materials and methods

Data for building DAYCENT models

The information about the study site and switchgrass field management was used as model input data for building DAYCENT models. The study site is located 45°16′24.55″ N, 97°50′13.34″ W (altitude: 524.3 m above sea level), near Bristol, South Dakota, USA. It was arranged into 12 plots (each plot is 21.3 m wide and 365.8 m long) with 2–20% slope. The plots were laid out in a split-plot design comprised of three N fertilization rates (low, 0 kg N ha$^{-1}$; medium, 56 kg N ha$^{-1}$; and high, 112 kg N ha$^{-1}$) and two landscape positions (shoulder and footslope). Switchgrass (cultivar: sunburst; planting rate: 10 kg pure live seed (PLS) ha$^{-1}$) was planted on May 17, 2008. Switchgrass was harvested once annually around a killing frost the year after establishment from 2009 to 2015. The previous crop grown on the plots was soybean. The mean annual precipitation and the mean daily temperature from 1986 to 2015 were 619 mm and 6.42 °C, respectively. The soils at the site are dominated by loamy soils (Mbonimpa et al., 2015b).

Other modeling input data were extracted from various sources. Soil texture data were obtained from the USDA-NCSS soil survey (SoilWeb, 2014). The measured $\rho_s$ and soil pH data from 2009 to 2013 were retrieved from the dissertation by Lai (2017). Daily minimum and maximum temperature and precipitation data from 1956 to 2014 were retrieved from our previous publication (Lai et al., 2016) at the same study site, and the daily weather data in 2015 and 2016 were obtained from the nearest weather station based on the method described in the same publication (Lai et al., 2016).

The measured data for calibration and validation of DAYCENT models were extracted from various previously published papers at the same study site. The measured data of the soil NO$_3$ from 2009 to 2013 and the soil surface N$_2$O fluxes from 2010 to 2015 have been published in our previous study (Lai et al., 2017). The measured soil surface CO$_2$ fluxes data from 2010 to 2012 have been published in another study (Mbonimpa et al., 2015b), and the CO$_2$ fluxes data for 2014 and 2015 were measured based on the same method described in the same study (Mbonimpa et al., 2015b). The measured SOC data from 2009 to 2013 were retrieved from the dissertation by Lai (2017). The switchgrass biomass yield data from 2009 to 2012 were obtained from the previous publication (Hong et al., 2014), and the yield data from 2013 to 2015 were measured based on the same method described in the same study (Hong et al., 2014). The measured yield values were averaged across three N rates and each year from 2009 to 2015 for this study. The WFPS values were calculated based on the measured soil bulk density using the equation mentioned below as:

$$WFPS = \frac{\theta}{\text{porosity}} \times 100, \text{porosity} = 1 - \frac{\rho_s}{\rho_b}$$  (1)

where WFPS is soil water-filled pore space (%), porosity (%) is soil porosity (%), $\theta$ is soil volumetric moisture content (cm$^3$ cm$^{-3}$), $\rho_s$ is soil particle density (2.65 g cm$^{-3}$), and $\rho_b$ is soil bulk density (g cm$^{-3}$) (NRCS, 2014a).

The two future scenarios S2 and S4 of climate change from 2016 to 2050 were generated using the global climate models in response to the intermediate emissions scenario 2 under the Representative Concentration Pathway (RCP) 4.5 W m$^{-2}$ and the high emissions scenario 4 under the RCP 8.5 W m$^{-2}$, respectively (Moss et al., 2008), based on the information such as latitude and longitude and altitude at the study site.

Establishment of DAYCENT models and prediction of soil parameters

The DAYCENT model Stand-alone Version DailyDayCent 08/17/2014 was used for predicting the selected parameters that include the following: SOC, NO$_3$, WFPS, CO$_2$ and N$_2$O fluxes, and biomass yield. DAYCENT models were built separately for CO$_2$ and N$_2$O fluxes using the measured soil surface CO$_2$ and N$_2$O fluxes, respectively, in response to six different treatments based on the three N rates and two positions. The six CO$_2$ models were built using the measured CO$_2$ flux data from 2010 to 2012 under high N rate at shoulder (M1), medium N rate at shoulder (M2), low N rate at shoulder (M3), high N rate at footslope (M4), medium N rate at footslope (M5), and low N rate at footslope (M6). Similarly, the six N$_2$O models were built using the measured N$_2$O flux data from 2010 to 2012 for high N rate at shoulder (M7), medium N rate at shoulder (M8), low N rate at shoulder (M9), high N rate at footslope (M10), medium N rate at footslope (M11), and low N rate at footslope (M12).

The model input data included daily precipitation and maximum and minimum temperature, soil texture, soil bulk density, pH, historical land use and field and crop management, and site information for building the 12 models. Calibration and validation of the DAYCENT models were conducted using the CPTE [Combined Parameter estimation (PEST) model (Doherty, 1994) and Trial-Error method] methodology, which is an improved method for the model calibration and validation. The methodology combined the Trial-Error and PEST model, an inverse modeling method, to overcome the drawbacks of either Trial-Error or PEST model method alone for the model calibration and validation. The detail of the improved methodology was described in our previous studies (Mbonimpa et al., 2015a; Lai et al., 2016). For the CO$_2$ models (M1-M6), the measured CO$_2$ fluxes in 2010–2012 were used for the calibration and the data in 2014–2015 were used for the validation, while the soil temperature and moisture, WFPS, SOC, and yield were further used to validate the models. For the N$_2$O models (M7-12), the N$_2$O fluxes in 2010–2012 were used for the calibration and the
data in 2014–2015 were used for the validation, while the soil temperature and moisture, WFPS, NO$_3^-$, and yield were used to further validate the models.

The calibrated and validated M1-6 models were used to predict the daily SOC, WFPS, and CO$_2$ flux in response to the two future climate scenarios S2 and S4. The calibrated and validated M7-12 models were used to predict the daily soil N$_2$O flux, NO$_3^-$ content, and annual switchgrass biomass yield in response to the S2 and S4 scenarios. The switchgrass growing season for each year was from May to October, and thereby, all the GHG data were calculated based on the growing season (May through October) for each predicted year.

**Evaluation of DAYCENT model performance and statistical analysis**

The model performance for the calibration and validation was evaluated based on the four criteria that include the coefficient of determination ($R^2$), percent bias (PBIAS; Gupta et al., 1999), model performance efficiency (ME; Nash & Sutcliffe, 1970), and RSR [the ratio of the root mean square error (RMSE) to standard deviation (SD) of the measured data] (Singh et al., 2005). The acceptable ranges are $0.5 \leq R^2 \leq 1$, $-15\% \leq \text{PBIAS} \leq +15\%$, $0.5 \leq \text{ME} \leq 1$, and $0 \leq \text{RSR} \leq 0.70$ (Moriasi et al., 2007). In general, the performance of model simulation can be judged as satisfactory if $R^2$, PBIAS, ME, and RSR are in their acceptable ranges (Moriasi et al., 2007).

The impacts of N rate, landscape position, and future climate change scenario on the predicted parameters were analyzed using analysis of variance (ANOVA) method. Data were transformed when necessary, and transformation was determined using the Box-Cox method (Box & Cox, 1964, 1981). Above statistical analyses were conducted using SAS9.4 (SAS, 2013). The data trend tests were conducted using the Mann-Kendall method (Mann, 1945; Kendall, 1975; Gilbert, 1987) with slopes estimated by the Sen Estimator (Sen, 1968) using the package ‘`mblm`’ in R (Komsta, 2013; R Core Team, 2016). Significance was determined at $\alpha = 0.05$ level for all statistical analyses in this study.

**Results**

**Calibration and validation of DAYCENT models**

The performance of calibration and validation of DAYCENT models, M1 through M12, is shown in Tables S1 and S2. The M1-6 models were calibrated using the measured CO$_2$ fluxes for 2010 through 2012. The $R^2$ values of M1-6 models were in the acceptable range of 0.50–1.00, indicating that there was a strong linear relationship between the modeled and measured CO$_2$ fluxes. The PBIAS values of M1-6 were in the acceptable range of $-15\%$ to $+15\%$, which signified that the means of the modeled and measured CO$_2$ fluxes were almost the same. The MEs of M1-6 were also in the acceptable range of 0.50–1.00 (note: the ME of M6 was 0.47, which is $-0.5$, thereby the M6 was also regarded as acceptable for this study). Furthermore, the RSR values of M1-5 were in the acceptable range of 0–0.70, indicating that the models had a smaller root mean square error. The RSR of M6 was 0.72, which is $-0.70$, the model was also acceptable (Table S1). These findings suggested that the simulations of calibrated M1-6 were satisfactory. Based on the same criteria, the M1-6 models were validated using the measured CO$_2$ data for 2014 through 2015 and observed the satisfactory simulation. The simulations of M1-6 were further validated using the measured soil temperature and moisture, WFPS, and yield data, and were also satisfactory. The results of M1-6 validated using the measured SOC density showed that the M1-3 and M5-6 were acceptable based on the results of PBIAS and $R^2$ for the purpose of prediction, but the M4 underestimated SOC density based on the low PBIAS ($-21.7\%$), which is out of the acceptable range of $-15\%$ to $15\%$ (Table S1).

The M7-12 models calibrated using the measured N$_2$O fluxes in 2010–2012 were satisfactory based on the same four criteria. The validations of models M7 through 12 using the N$_2$O fluxes in 2014–2015 showed that they were satisfactory for the purpose of prediction because their PBIASs were in the acceptable range. The model validation using the measured soil temperature and moisture, WFPS, and yield showed that the models were satisfactory. However, the soil NO$_3^-$ contents were underestimated by the models M7 through 9 and M12 due to their lower PBIAS values based on their validation results using the measured soil NO$_3^-$ contents (Table S2).

**Soil organic carbon (SOC) density**

Data for the predicted SOC density (kg m$^{-2}$) values for the 0- to 10-cm depth under different treatments from 2016 to 2050 are presented in Tables 1 and 2 and Fig. S1a,b. Because the interactions effect between the N rate and the position on the SOC density values from 2016 to 2050 under the S2 and S4 climate scenarios were statistically significant, the SOC data were separately analyzed for each N rate and position. For the S2 and S4 scenarios, under each N rate, the SOC density at the footslope position was significantly higher than that of the shoulder position. At the shoulder, the SOC density values under the high and low N rates were significantly higher than that of the medium N rate. At the footslope position, the SOC density under the high N rate was significantly higher than that for the medium N rate, which was significantly higher than the low N rate. For each N rate and position, the SOC density values under the S2 and S4 scenarios were not significantly different. The values of SOC density for the N rate and position under the S2 and S4 were in the range of 1.81–3.12 kg m$^{-2}$ (Table 1).

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For both the S2 and S4 scenarios, Kendall trend tests indicated significant upward trends in the SOC density values under the high N rate at the shoulder and footslope positions from 2016 to 2050 ($P < 0.05$ with positive slopes) except for the SOC density under the high N rate at the shoulder for the S2, where no significant trend was detected ($P = 0.16$). The trend test also indicated that there was a significant downward trend in the SOC density at the shoulder position ($P < 0.05$ with negative slopes). Moreover, significant downward trends in the SOC density values were detected under the low N rate at the shoulder and footslope positions over the years ($P < 0.05$ with negative slopes) (Table 2 and Fig. S1a,b).

### Soil nitrate (NO$_3$) Content

Data on the predicted NO$_3$ contents (mg kg$^{-1}$) at the 5- to 10-cm depth under different treatments from 2016 to 2050 are presented in Tables 2 and 3 and Fig. S2a,b. The effects of interactions between the N rate and the position on the soil NO$_3$ contents in 2016–2050 under the S2 and S4 climate scenarios were statistically significant, and therefore, the NO$_3$ data were separately analyzed for each N rate and position. The simulated results showed that under the high and medium N rates for the S2 and S4 scenarios, NO$_3$ contents at the footslope position were significantly higher than that for the shoulder position. Under the low N rate, the NO$_3$ contents at the footslope position were significantly lower than the footslope position under the S4, and the NO$_3$ contents at the shoulder and footslope positions for the S2 were not significantly different. At the shoulder and footslope positions for the S2 and S4 scenarios, the NO$_3$ content under the high N rate was significantly higher than that for the medium N rate, which was significantly higher than that under the low N rate. For each N rate and position, the NO$_3$ content under the S2 was significantly higher than that under the S4. The highest value of NO$_3$ content among the interactions between the N rate and position for the S2 and S4 scenarios was 11 mg kg$^{-1}$ (under the high N rate at the footslope for the S2), and the lowest was 0.63 mg kg$^{-1}$ (under the low N rate at the footslope position for the S4) (Table 3).

Kendall trend tests indicated significant downward trends in the NO$_3$ contents under the low N rate at the shoulder and footslope positions for the S2 scenario from 2016 to 2050 ($P < 0.05$ with negative slopes). However, no significant trend in the NO$_3$ content was detected under the high and medium N rates at the shoulder and footslope positions for the S2 scenario ($P > 0.05$). Under the S4 scenario, the trend tests denoted significant upward trends in the NO$_3$ contents under the high and medium N rates at the shoulder and footslope positions over the years ($P < 0.05$ with positive slopes) and significant downward trends in the NO$_3$ contents under the low N rate at the shoulder and footslope positions for the period ($P < 0.05$ with negative slopes) (Table 2 and Fig. S2a,b).

### Soil water-filled pore space (WFPS)

The predicted WFPS (%) data at the 5- to 10-cm depth under different treatments from 2016 to 2050 are

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**Table 1** DAYCENT predicted mean soil organic carbon (SOC) density values in the 0- to 10-cm depth from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4

| Treatments | SOC (kg m$^{-2}$) |
|------------|------------------|
|            | S2*              | S4*              |
| N Rate     |                  |                  |
| High       | 2.72$^{aA}$      | 2.77$^{A}$       |
| Medium     | 2.25$^{bA}$      | 2.28$^{A}$       |
| Low        | 2.43$^{bB}$      | 2.44$^{B}$       |
| Position   |                  |                  |
| Shoulder   | 2.18$^{bB}$      | 2.20$^{bA}$      |
| Footslope  | 2.76$^{bA}$      | 2.80$^{A}$       |

Analysis of variance ($P > F$)

| N Rate     | Position | N Rate × Position$^2$ |
|------------|----------|----------------------|
|            |          |                      |
|            | S2       | S4                   |
| Shoulder   |          |                      |
| High       | 2.39$^{bB}$ | 3.06$^{aA}$           |
| Medium     | 1.81$^{bB}$ | 2.68$^{bA}$           |
| Low        | 2.33$^{bB}$ | 2.53$^{aA}$           |

$^*$S2 represents future climate scenario 2, which is in response to the intermediate emissions scenario 2 (RCP4.5 W m$^{-2}$). S4 denotes future climate scenario 4, which is in response to the high emissions scenario 4 (RCP8.5 W m$^{-2}$). RCP, Representative Concentration Pathway.

$^1$Means within the same column followed by different small letters are significantly different at $P < 0.05$ for the N rate and position. Means within the same row followed by different capital letters are significantly different at $P < 0.05$ for the climate scenario.

$^2$This is the results that the data were analyzed separately for each N rate and position because of the $P$ values of N rate × Position < 0.05.
Table 2  Trend test P-values and trend slopes of the DAYCENT predicted (based on two future climate scenarios S2 and S4) mean SOC density, soil NO\textsubscript{3}, WFPS, and CO\textsubscript{2} and N\textsubscript{2}O fluxes for 2016–2050 under switchgrass field managed with the high, medium, and low N rates at the shoulder and footslope positions

| Treatment | Trend test* | SOC       | NO\textsubscript{3} | WFPS     | CO\textsubscript{2} | N\textsubscript{2}O |
|-----------|-------------|-----------|---------------------|----------|---------------------|---------------------|
| Climate Scenario S2† |             |           |                     |          |                     |                     |
| Shoulder  |             |           |                     |          |                     |                     |
| High      | P-value     | 0.16      | 0.21                | <0.001   | <0.001              | <0.001              |
|           | Slope       | 0.0005    | 0.0098              | –0.0380  | 0.0138              | 0.0350              |
| Medium    | P-value     | <0.001    | 0.67                | 0.01     | <0.001              | <0.001              |
|           | Slope       | –0.0046   | 0.0004              | –0.0300  | 0.0134              | 0.0181              |
| Low       | P-value     | <0.001    | <0.001              | <0.001   | <0.001              | <0.001              |
|           | Slope       | –0.0075   | –0.0030             | –0.0540  | –0.0146             | –0.0150             |
| Footslope |             |           |                     |          |                     |                     |
| High      | P-value     | <0.001    | 0.84                | <0.001   | <0.001              | 0.98                |
|           | Slope       | 0.0326    | –0.0005             | –0.0340  | 0.0187              | –0.0016             |
| Medium    | P-value     | 0.002     | 0.75                | 0.01     | <0.001              | 0.24                |
|           | Slope       | 0.0025    | –0.0010             | –0.0362  | 0.0077              | 0.0021              |
| Low       | P-value     | <0.001    | <0.001              | <0.001   | <0.001              | <0.001              |
|           | Slope       | –0.0075   | –0.0030             | –0.0540  | –0.0146             | –0.0150             |
| Climate Scenario S4† |             |           |                     |          |                     |                     |
| Shoulder  |             |           |                     |          |                     |                     |
| High      | P-value     | <0.001    | <0.001              | <0.001   | <0.001              | <0.001              |
|           | Slope       | 0.0050    | 0.0120              | –0.0391  | 0.0223              | 0.0310              |
| Medium    | P-value     | <0.001    | <0.001              | <0.001   | 0.01                | 0.01                |
|           | Slope       | –0.0022   | 0.0052              | –0.1194  | 0.0184              | 0.0047              |
| Low       | P-value     | <0.001    | <0.001              | <0.001   | 0.01                | <0.001              |
|           | Slope       | –0.0068   | –0.0150             | –0.0375  | –0.0029             | –0.0163             |
| Footslope |             |           |                     |          |                     |                     |
| High      | P-value     | <0.001    | 0.002               | <0.001   | <0.001              | 0.21                |
|           | Slope       | 0.0052    | 0.0095              | –0.0440  | 0.0188              | 0.0046              |
| Medium    | P-value     | <0.001    | <0.001              | <0.001   | 0.01                | 0.11                |
|           | Slope       | 0.0048    | 0.0089              | –0.0661  | 0.0109              | 0.0097              |
| Low       | P-value     | <0.001    | <0.001              | <0.001   | 0.01                | <0.001              |
|           | Slope       | –0.0068   | –0.0025             | –0.0375  | –0.0029             | –0.0163             |

*P-values were from the results of trend tests using the Mann-Kendall method. Slopes were estimated using the Sen Estimator.
†Climate scenario S2 is in response to the intermediate emissions scenario 2 (RCP4.5 W m\textsuperscript{−2}). Climate scenario S4 is in response to the high emissions scenario 4 (RCP8.5 W m\textsuperscript{−2}). RCP, Representative Concentration Pathway.

presented in Tables 2 and 4 and Fig. S3a,b. The effects of interaction between the N rate and the position on the WFPS values in 2016–2050 under the S2 and S4 scenarios were significant; thus, the WFPS data were separately analyzed for each N rate and landscape position. For the S2 and S4 scenarios, under each N rate, the WFPS at the shoulder was significantly higher than that at the footslope. At the shoulder, the WFPS under the high N rate was significantly higher than the medium N rate. At the footslope, the WFPS under the medium N rate was significantly higher than the high and low N rates. For each N rate and position, the WFPS under the S2 was significantly higher than that under the S4. The highest value of WFPS among the interactions between the N rate and position for the S2 and S4 scenarios was 51.9% (under the high N rate at the shoulder for the S2), and the lowest was 38.7% (under the high N rate at the footslope for the S4) (Table 4). Kendall trend analyses indicated significant downward trends in the WFPS values for all treatments from 2016 to 2050 (P < 0.05 with negative slopes) (Table 2 and Fig. S3a,b).

Soil surface carbon dioxide (CO\textsubscript{2}) fluxes

The predicted mean soil surface CO\textsubscript{2} fluxes (g m\textsuperscript{−2} d\textsuperscript{−1}) under different treatments from 2016 to 2050 are presented in Tables 2 and S3 and Fig. 1a–f. The effects of interaction between the N rate and the landscape position on the predicted mean CO\textsubscript{2} fluxes for the switchgrass growing season from 2016 to 2050 for the S2 and S4 scenarios were significant; thus, the CO\textsubscript{2} data were separately analyzed for each N rate and position. For the S2 and S4 scenarios, under the high and low N
rates, the CO2 fluxes at the footslope were significantly higher than the shoulder, whereas, under the medium N rate, the CO2 fluxes at the footslope and shoulder positions were not significantly different. At the shoulder for the S2, the CO2 fluxes under the low N rate were significantly higher than the medium N rate, whereas, for the S4, the CO2 fluxes under the three N rates were not significantly different. At the footslope for the S2 and S4 scenarios, the CO2 fluxes under the medium N rate were significantly lower than the high and low N rates. For each N rate and position, the CO2 fluxes at the footslope were significantly higher than the shoulder, whereas, under the medium N rate, the CO2 fluxes under the three N rates were not significantly different.

### Table 3 DAYCENT predicted mean soil NO3 contents in the 5- to 10-cm depth from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4

| Treatments | Soil NO3 (mg kg⁻¹) |
|------------|-------------------|
|            | S2*               | S4*               |
| **N Rate** |                   |                   |
| High       | 9.17±A1           | 9.02±B           |
| Medium     | 2.72±A1           | 2.63±B           |
| Low        | 0.68±A            | 0.65±B           |
| **Position** |               |                   |
| Shoulder   | 3.29±A            | 3.22±B           |
| Footslope  | 5.09±A            | 4.98±B           |

Analysis of variance (P > F)

| N Rate x Position | S2 | S4 |
|-------------------|----|----|
| N Rate            | <0.001 | <0.001 |
| Position          | <0.001 | <0.001 |
| N Rate x Position | <0.001 | <0.001 |

* S2 represents future climate scenario 2, which is in response to the intermediate emissions scenario 2 (RCP4.5 W m⁻²). S4 denotes future climate scenario 4, which is in response to the high emissions scenario 4 (RCP8.5 W m⁻²). RCP, Representative Concentration Pathway.

1 Means within the same column followed by different small letters are significantly different at P < 0.05 for the N rate and position. Means within the same row followed by different capital letters are significantly different at P < 0.05 for the climate scenario.

2 This is the results that the data were analyzed separately for each N rate and position because of the P values of N rate x Position < 0.05.

### Table 4 DAYCENT predicted mean soil water-filled pore space (WFPS) values in the 5- to 10-cm depth from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4

| Treatments | WFPS (%) |
|------------|----------|
|            | S2*      | S4*      |
| **N Rate** |          |          |
| High       | 46.03±AB  | 44.28±B  |
| Medium     | 46.41±A   | 44.83±B  |
| Low        | 45.57±A   | 44.06±B  |
| **Position** |        |          |
| Shoulder   | 51.00±A   | 49.38±B  |
| Footslope  | 41.01±B   | 39.40±B  |

Analysis of variance (P > F)

| N Rate x Position | S2 | S4 |
|-------------------|----|----|
| N Rate            | 0.002 | <0.001 |
| Position          | <0.001 | <0.001 |
| N Rate x Position | <0.001 | <0.001 |

* S2 represents future climate scenario 2, which is in response to the intermediate emissions scenario 2 (RCP4.5 W m⁻²). S4 denotes future climate scenario 4, which is in response to the high emissions scenario 4 (RCP8.5 W m⁻²). RCP, Representative Concentration Pathway.

1 Means within the same column followed by different small letters are significantly different at P < 0.05 for the N rate and position. Means within the same row followed by different capital letters are significantly different at P < 0.05 for the climate scenario.

2 This is the results that the data were analyzed separately for each N rate and position because of the P values of N rate x Position < 0.05.
Soil surface nitrous oxide (N₂O) fluxes

The predicted soil surface N₂O fluxes (g ha⁻¹ d⁻¹) data under different treatments from 2016 to 2050 are presented in Tables 2 and S4 and Fig. 2a–f. The effects of interaction between the N rate and the position on the predicted mean N₂O fluxes during the growing season for 2016–2050 under the S2 and S4 scenarios were statistically significant, and thereby, the N₂O data were separately analyzed for each N rate and position. For the S2 and S4 scenarios, under the high and low N rates, the N₂O fluxes at the footslope were significantly higher than that at the shoulder, whereas, under the medium N rate, the N₂O fluxes at the footslope were significantly lower than the shoulder. At the shoulder, the N₂O flux under the medium N rate was significantly higher than that for the high N rate, which was significantly higher than that under the low N rate. At the footslope, the N₂O flux under the high N rate was significantly higher than the medium N rate, which was significantly higher than the low N rate. Under the high N rate at the shoulder and footslope positions, the N₂O fluxes under the S2 were significantly higher than the S4, but under the medium and low N rates, the N₂O fluxes under the S2 and S4 scenarios were not significantly different. The highest value of mean N₂O flux was 4.17 g ha⁻¹ d⁻¹ under the medium N rate at the shoulder for the S2, and the lowest was 1.66 g ha⁻¹ d⁻¹ under the low N rate at the shoulder for the S4 (Table S4). Kendall trend tests denoted significant upward trends in the N₂O fluxes under the high and medium N rates at the shoulder position from 2016 to

![Figure 1](image-url)
2050 ($P < 0.05$ with positive slopes). However, no significant trend in the $\text{N}_2\text{O}$ fluxes was detected under the high and medium $N$ rates at the footslope position. Moreover, the trend tests indicated significant downward trends in the $\text{N}_2\text{O}$ fluxes under the low $N$ rate at the shoulder and footslope positions over the years ($P < 0.05$ with negative slopes) (Table 2 and Fig. 2a–f).

Discussion

DAYCENT simulated impacts of $N$ fertilization rate on soils and the environment

The findings from this study showed that the SOC density values at the shoulder position under the high and low $N$ rates were significantly higher than those of the medium $N$ rate, and the SOC density values at the footslope position under the high $N$ rate were significantly higher than the medium and low $N$ rates (Table 1). The impact of the $N$ rate on SOC density at the footslope position is in accord with some previous studies that showed that the fertilizer additions increased the SOC and root C storage (e.g., Blanco-Canqui, 2010; Schmer et al., 2011). However, the impact at the shoulder position differs from above studies. This could be because the water erosion resulting from the switchgrass land with slope disturbed and/or redistributed SOC at the shoulder position. In the process of water erosion, SOC in the loose surface soil (part of the SOC results from the application of $N$ fertilizer) is first transported

Figure 2  Trends of the predicted mean growing season soil $\text{N}_2\text{O}$ fluxes under the high, medium, and low $N$ rates at the shoulder for the S2 (a) and for the S4 (b), at the footslope for the S2 (c) and for the S4 (d), and the mean at the shoulder and footslope positions for the S2 (e) and the S4 (f) in the switchgrass field from 2016 to 2050. S2 represents future climate scenario 2, which is in response to the intermediate emissions scenario 2 (RCP4.5 W m$^{-2}$). S4 denotes future climate scenario 4, which is in response to the high emissions scenario 4 (RCP8.5 W m$^{-2}$). RCP, Representative Concentration Pathway.

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(Polyakov & Lal, 2004). Then, the sediment repeatedly removed could mix the topsoil and subsoil, reducing the SOC content in the eroded soils (Martínez-Mena et al., 2012). Sediment-enriched SOC, however, is not obvious in the low SOC content of the original soils (Zhang et al., 2013). Therefore, more SOC in the soils with the higher N fertilization rates may be removed than that in the original soil (not disturbed, i.e., under the low N rate in this study), resulting in that the SOC density under the medium N rate could be lower than that for the low N rate at the shoulder position. Although the SOC density values were underestimated by the two DAYCENT models M4 and M6 (PBIASs were lower as shown in Table S1), this may not affect the assessment of the impacts of growing switchgrass because their time trends and magnitude order among the treatments were not changed.

Soil NO$_3^-$ contents under the high N rate were significantly higher than that for the medium and low N rates at the shoulder and footslope positions (Table 3), which is in accord with some previous studies (e.g., Jokela, 1992; Abalos et al., 2014). The N fertilizer is one of the major sources of soil NO$_3^-$ supply (Schimel & Bennett, 2004). The NH$_4^+$ fertilizer is rapidly converted to NO$_3^-$ by autotrophic bacteria and archaea (Whalen & Sampedro, 2010). The continuous application of N fertilizer can result in more soil NO$_3^-$ contents, especially the higher N rate lead to higher soil NO$_3^-$ content. Furthermore, the NO$_3^-$ contents under each N rate were underestimated by the four DAYCENT models (PBIASs were lower as shown in Table S2). However, this may not influence the assessment of evaluating the impacts of growing switchgrass on NO$_3^-$ contents because the time trends and order of magnitudes of NO$_3^-$ contents under various treatments were not changed.

At the shoulder, the WFPS under the high N rate was significantly higher than that for the medium N rate. However, at the footslope, the WFPS under the medium N rate was significantly higher than the high and low N rates (Table 4). The WFPS, in general, decreases with the increase in N rate because of decreased $\rho_b$ with the increase in N rate (Murphy et al., 2004; Blanco-Canqui, 2010). However, the WFPS is also influenced by rainfall through impacting soil volumetric water content ($\theta$). The rainfall is an uncertain or variable factor of climate. Therefore, the WFPS values among different N rates could not follow the increased trend with the increase in N rate.

At the shoulder position under the S2 climate scenario, the CO$_2$ fluxes under the low N rate were significantly higher than for the medium N rate, whereas the CO$_2$ fluxes under the three N rates for the S4 scenario were not significantly different. At the footslope position for both the S2 and S4 scenarios, the CO$_2$ fluxes under the medium N rate were significantly lower than those of the high and low N rates (Table S3). Some previous studies have also documented that the N fertilizer applied to switchgrass had different effects on soil CO$_2$ emissions. For example, Schmer et al. (2012) found that the N fertilization did not impact soil CO$_2$ emissions in the Northern Great Plains. However, another study showed that the N rate did not impact soil CO$_2$ emissions in 2010 and 2011, but impacted the CO$_2$ emissions in the summer of 2012 in South Dakota (Mbonimpa et al., 2015b). These diverse findings in this study may be due to different impacts of multifactors on soil CO$_2$ fluxes. The autotrophic (e.g., plant roots) and heterotrophic (e.g., soil microbes) respirations are the two major ways in plant–soil systems those are contributing to atmospheric CO$_2$ (Amacher & Mackowiak, 2011). Soil can act as both source and sink of atmospheric CO$_2$ (Sainju et al., 2006). The decrease in SOC due to water erosion can reduce soil CO$_2$ fluxes (Wang et al., 2014). Higher WFPS or $\rho_b$ can result in lower porosity based on the Eqn (1), reducing aerobic conditions and restricting CO$_2$ diffusivity from soils (Bearé et al., 2009). Temperature and precipitation strongly impact the soil CO$_2$ emissions, and the optimal conditions for the respiration are when soil macropores are filled with air and micropores with water (Davidson et al., 2000). The lower SOC, higher bulk density, and higher WFPS at the shoulder position than the footslope position during the growing season (Mbonimpa et al., 2015b) could result in different CO$_2$ fluxes from soils under the same N rates at the shoulder and footslope positions under the two climate scenarios.

Soil surface N$_2$O fluxes under the high N rate were significantly higher than that under the medium and low N rates at the footslope position (Table S4). This is in accord with a previous study conducted by Schmer et al. (2012). However, at the shoulder position, the N$_2$O flux under the medium N rate was significantly higher than that for the high N rate, which was significantly higher than that under the low N rate (Table S4). This also differs from other studies. For example, Nikiéma et al. (2011) reported no differences in N$_2$O fluxes between the N fertilizer applications compared with the unfertilized switchgrass. Wile et al. (2014) found that the N fertilizer effect on N$_2$O emissions was significant for 2008 but not for 2009 in Canada. These different findings in the present study could be due to the interacted impacts of various factors on N$_2$O flux. Based on some findings from the previous studies (Lin et al., 2000; Parton et al., 2001; Tian et al., 2010a,b), the N$_2$O flux is a function of soil temperature ($t$), $\theta$, soil porosity, net N mineralization ($\text{Net}_{\text{min}}$) from the soil organic matter (SOM) decomposition, soil NH$_4^+$ concentration,
WFPS, pH, $\rho_b$, soil gas diffusivity ($D/D_0$, which is a function of WFPS, $\rho_b$, and $\theta$ at field capacity), and heterotrophic respiration (note: the rates of nitrification and denitrification in soils are also determined by these parameters; Lai et al., 2017). The parameters $t$ and $\theta$ are not associated with N rate, the NH$_4$ usually does not accumulate in the soils (Woodruff & Ruger, 1948). The N rate, however, can increase SOC and TN at the top depth after continuous N fertilizer application (Blanco-Canqui, 2010; Schmer et al., 2011), impacting the Net$_{min}$, WFPS, pH, $\rho_b$, and heterotrophic respiration. The effects of N rate on SOC and NO$_3^-$ were same [i.e., the higher N rates resulted in the higher SOC and NO$_3^-$ contents (Tables 1 and 3)] at the footslope position. These can enhance denitrification rate ($N_{denit}$) under the higher N rates than the lower N rate (Chantigny et al., 1998; Luce et al., 2011), resulting in the N$_2$O fluxes under the higher N rate were higher than that for the lower N rate at the footslope (Table S4). However, at the shoulder position, the effects of N rate on SOC and NO$_3^-$ were different (Tables 1 and 3), likely resulting in higher N$_2$O fluxes under the medium N rate, compared with the high N rate (Table S4).

Furthermore, the N rate significantly impacted switchgrass yield. At the shoulder position, the biomass yield of switchgrass under the high and medium N rates was significantly higher than that of the low N rate. At the footslope position, the yield under the high N rate was significantly higher than the medium N rate, which was significantly higher than the low N rate (Table S5). The yield under the high and medium N rates had an upward trend from 2016 to 2050, but the yield under the low N rate followed a downward trend (Fig. S4a,b). The data showed that the medium N fertilization was considered as the best rate for the switchgrass production both economically (higher biomass yield) and environmentally (higher CO$_2$ and N$_2$O fluxes).

Model simulated impacts of topography on soils and the environment

The findings from this study showed that, in general, under each N rate, the landscape topography significantly impacted the SOC, NO$_3^-$, WFPS, and CO$_2$ and N$_2$O fluxes. The SOC density, NO$_3^-$ content, and CO$_2$ and N$_2$O fluxes at the footslope position were mostly significantly higher than those of the shoulder position, and the WFPS at the footslope position was significantly lower than the shoulder position (Tables 1, 3, 4, S3, and S4). The results are in accord with those reported previously (e.g., Ofori et al., 2013; Mbonimpa et al., 2015b). The topography can result in soil erosion and change the SOM distribution (Guzman & Al-Kaisi, 2011). The shoulder position is generally eroded while the depositions occur at the footslope position (McCarty & Ritchie, 2002). Most of the soil nutrients are accumulated at the footslope position (Papiernik et al., 2007), and thereby, the SOC density and NO$_3^-$ contents are usually higher at the footslope than the shoulder. This can result in an increase in root biomass and soil aggregation at the footslope position, and soil degradation at the shoulder position. The increase in the SOM, soil structure, and root biomass at the footslope position can primarily contribute to decreased $\rho_b$ (Guzman & Al-Kaisi, 2011), which increase WFPS at the footslope position (NRCS, 2014a). Also, the increase in SOM and root biomass at the footslope position can increase the heterotrophic (majorly from soil microbes) and the autotrophic (mainly from plant roots) respiration, respectively, subsequently increasing the CO$_2$ fluxes at the footslope position. Furthermore, the increase in SOC and NO$_3^-$ contents at the footslope position can enhance the rate of denitrification (Helgason et al., 2005; Luce et al., 2011), resulting in higher N$_2$O fluxes at the footslope, compared with the shoulder position.

Modeled impacts of climate change on soils and the environment

The annual mean air temperature under the S4 scenario is greater than that of the S2 scenario, but the annual precipitation under the S4 is <S2 (Fig. S5). The temperature and precipitation directly determine the level of soil temperature and moisture, respectively (Kutsch et al., 2009; Subke & Bahn, 2010). The findings from this study showed that climate scenario significantly impacted NO$_3^-$, WFPS, and N$_2$O fluxes, but did not impact SOC and CO$_2$ fluxes (Tables 1, 3, 4, S3, and S4). The NO$_3^-$ contents under the S2 were significantly higher than the S4 for each N rate and position (Table 3). This was because the soil NO$_3^-$ was continually supplied through the natural processes of mineralization and nitrification of SOM (Randall & Mulla, 2001), in which the appropriate conditions of soil temperature and moisture may facilitate higher rates of mineralization and nitrification of SOM in the plant–soil systems under the S2 than the S4. The WFPS values under the S2 were significantly higher than that under the S4 for each N rate and position (Table 4). This was because (i) the precipitation under the S2 was higher than that for the S4 (Fig. S5), resulting in higher soil moisture for the S2, and (ii) the temperature under the S2 was lower than that for the S4, leading to lower soil moisture for the S4 through increasing evapotranspiration with the increasing soil temperature (Liu et al., 2009; Poll et al., 2013).
The soil N$_2$O fluxes under the S2 scenario were significantly higher than that for the S4 scenario under the high N rate or at the shoulder and footslope positions (under the medium and low N rates, the N$_2$O fluxes under the S2 and S4 scenarios were not significantly different; Table S4). This differs from the study by Abdalla et al. (2010) who reported that the soil surface N$_2$O fluxes were not projected to increase significantly under the climate change (both high- and low-temperature sensitivity scenarios). The N$_2$O emissions from soils are mainly generated in the two processes: denitrification and nitrification (Verstraete & Focht, 1977), and the denitrification is the principal pathway to produce the N$_2$O emissions into the atmosphere (Weier et al., 1993). The denitrification rate is affected by the climate change and temperature or their interaction function through impacting soil NO$_3^-$, SOM decomposition, WFPS, and crop growth (Conant et al., 2011; Glenn et al., 2012). As stated previously, the NO$_3^-$ contents under the S2 were significantly higher than that under the S4 for each N rate and position (Table 3). This could result in higher N$_2$O fluxes under the S2 than the S4 via denitrification where denitrifying bacteria use NO$_3^-$ instead of oxygen (Luce et al., 2011; Lai et al., 2017). Also, because the WFPS under the S2 was significantly higher than that under the S4 for each N rate and position (Table 4), the higher WFPS can result in higher N$_2$O fluxes under the S2 than the S4 based on the equation $N_{\text{denit}} = 0.5 \tan (0.6\pi (0.1 \times \text{WFPS} - a))/\pi$, where $a$ is a function of soil gas diffusivity and heterotrophic respiration (Parton et al., 2001).

Summarily, the S4 scenario significantly reduced the soil NO$_3^-$ and WFPS, compared with the S2 scenario (Tables 3 and 4), indicating the interaction of higher temperature and lower precipitation (S4) could undermine the soil fertility. However, the climate change under the S4, compared with the S2, did not significantly increase CO$_2$ fluxes for each N rate and significantly decreased N$_2$O fluxes under the high N rate and the two positions, indicating the S4 could result in less GHG emissions under switchgrass fields.

**Trends in predicted parameters and time effects**

The findings from this study showed that the significant trends were observed for the most selected parameters under different N rates from 2016 to 2050 ($P < 0.05$) based on Kendall trend tests (Table 2). The SOC density under the high and medium N rates had an upward trend, whereas, under the low N rate, it showed a downward trend (Table 2 and Fig. S1a,b). This could be attributed to the switchgrass production, N fertilization, and climate factors. The switchgrass is a perennial plant that has an extensive fibrous root system, contributing organic matter to the soils (Brown et al., 2000; Frank et al., 2004). This can help in accumulating more SOC in the soils with low initial SOC contents under perennial energy crops over time (Kibet et al., 2016), resulting in the upward trend. Moreover, the N fertilization can encourage the growth of plant including below and above ground growth. Thus, the continuous N fertilization can further help in increasing or maintaining the SOC contents over time (Malhi et al., 2003; NRCS, 2014b). However, under the low N rate, no N fertilizer was applied, this could not increase and maintain the SOC contents and boost root growth, likely resulting in a downward trend in SOC density. Additionally, the increasing temperature and fluctuation of precipitation over the predicted years could reduce SOC contents in soils (Jobbágy & Jackson, 2000), resulting in a downward trend in SOC density under the low N rate over the predicted years.

Soil NO$_3^-$ contents under the high and medium N rates for the S4 scenario had a significant upward trend but no significant trend for the S2 scenario, and those under the low N rate had a significant downward trend for 2016–2050 (Table 2 and Fig. S2a,b). This could result from the interactions of multiple factors. As mentioned previously, the soil NO$_3^-$ is supplied by N fertilizer and taken up by plants, and it can leach into underground water and be converted into N$_2$O emissions through denitrification (Luce et al., 2011). Also, the natural processes of mineralization and nitrification of SOM can continually supply NO$_3^-$ for soils (Randall & Mulla, 2001). Switchgrass deep rooting system with the abundant and dense network (Clark et al., 1998; Blanco-Canqui, 2010) could have more arbuscular mycorrhizal (AM) fungi, which can increase N mineralization from SOM and availability of N (Jackson et al., 2008). However, the downward trend in soil NO$_3^-$ contents under the low N rate (no input of N fertilizer) from 2016 to 2050 could be due to the continuous harvest without N fertilization over the years.

Significant upward trends in soil CO$_2$ fluxes under the high and medium N rates but a slight downward trend under the low N rate from 2016 to 2050 were observed (Table 2 and Fig. 1a–d). This was primarily because the increasing temperature over the predicted years could result in increased SOM decomposition and CO$_2$ emissions (Davidson & Janssens, 2006). There was also an increasing trend in the biomass yield under the high and medium N rates (Fig. S4a,b). The increased biomass can subsequently increase in C flow to the soil with increased temperature under optimal precipitation conditions (Kanerva et al., 2007), likely resulting in an upward trend in CO$_2$ emissions from soils.
Furthermore, the slopes of the trends in soil CO2 fluxes under the high and medium N rates at the landscape positions for the two climate scenarios varied in the range of 0.0077–0.0223 (Table 2), which were very small, indicating that the increased CO2 fluxes under the high and medium N rates from 2016 to 2050 could be not significant. However, under the low N rate, the plant biomass decreased over the years (Fig. S4a,b), resulting in decreased C flow to the soil over time and subsequent downward trend in CO2 fluxes over the predicted years.

No significant upward trend in N2O fluxes at the footslope position for each N rate from 2016 to 2050 was detected. However, at the shoulder position, the N2O fluxes under the high and medium N rates had a significant upward trend (Table 2 and Fig. 2a–d). The findings could be attributed to multiple factors and the environmental conditions. The switchgrass field at this study site has not been cultivated (no soil disturbance) and possesses root perennial and deep rooting system (Clark et al., 1998; Blanco-Canqui, 2010) that can increase the SOM concentrations (Thomas et al., 1996) and lower the $p_b$ (Clark et al., 1998) over the years. The increased SOM can increase Netmin, resulting in the increase in Nnut, whereas the decreased $p_b$ can reduce WFPS, reducing Nnut and Nden (Martin et al., 1998; Parton et al., 2001). The principal pathway of producing the N2O emissions is the denitrification (Bouwman, 1990; Weier et al., 1993). Therefore, the decreasing Nden, resulting from the decreased $p_b$ is the main factor in impacting soil N2O fluxes over the years, leading to an insignificant trend of soil N2O fluxes over the years. Furthermore, the deep roots of switchgrass add organic matter to the soils, increasing the porosity which can increase the water infiltration rate over time (Katsvairo et al., 2007). This could lead to more leaching of NO3− from topsoil over time, reducing the source of N for denitrifying bacteria over time to emit N2O from soils (Hofstra & Bouwman, 2005), likely resulting in no significant upward trend in N2O fluxes. The simulation results indicate that growing perennial switchgrass could reduce soil surface N2O fluxes over time. However, at the shoulder position, the switchgrass biomass yield was lower compared with the footslope position (Fig. S4), and the N fertilization rate was the same as the footslope, thereby the soil N as a source of N2O emissions could be higher at the shoulder than the footslope. This could result in an upward trend in soil N2O fluxes over time with continuous N fertilizer application. Furthermore, the slopes of the trends in soil N2O fluxes at shoulder position were 0.035 (high N rate) and 0.018 (medium N rate) for the S2 scenario and 0.031 (high N rate) and 0.0047 (medium N rate) for the S4 scenario (Table 2). The slopes were very small, indicating that the increased N2O fluxes under the high and medium N rates at the shoulder position from 2016 to 2050 could be not significant. The slopes also showed the much higher slopes under the medium N rate than the high N rate, signifying the increased N2O fluxes under the medium N rate were much lower than that for the high N rate.

Conclusions

The data from this study showed that the N fertilization can improve SOC and soil NO3− and increase switchgrass yield, but negatively impact the environment through increasing soil surface N2O and CO2 fluxes. The medium N fertilization is the best fertilization rate for the switchgrass production both economically and environmentally. The footslope position can be beneficial for the SOC, NO3−, and yield and the environment by sequestering more SOC than that of the shoulder, but also have a negative effect on the environment through producing more N2O and CO2 emissions. The increase in temperature and decrease in precipitation (S4 vs. S2) can reduce the soil NO3− contents, WFPS, and N2O fluxes. Switchgrass production can improve and maintain the SOC and NO3−, and have a decrease in soil N2O and CO2 fluxes under the low N rate and an insignificant increase in soil N2O and CO2 fluxes under the high and medium N rates over the predicted years. The findings from this study revealed that switchgrass can be a sustainable energy crop on marginally yielding lands for improving soils without significant negative impacts on the environment in South Dakota. The conclusions can provide valuable information to make policy that supports switchgrass as a viable alternative bioenergy feedstock. Future work is needed to conduct a systematical analysis using more parameters based on long-term measured data from the switchgrass land for evaluating switchgrass production ecological impacts.

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Supporting Information

Additional Supporting Information may be found online in the supporting information tab for this article:

Fig. S1. Trends of the predicted mean growing season SOC density in the 0- to 10-cm depth under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field from 2016 to 2050.

Fig. S2. Trends of the predicted mean growing season soil NO3− in the 5- to 10-cm depth under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field from 2016 to 2050.

Fig. S3. Trends of the predicted mean growing season WFPS in the 5- to 10-cm depth under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field from 2016 to 2050.

Fig. S4. Trends of the predicted annual switchgrass biomass yields under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field from 2016 to 2050.

Fig. S5. Trends of the simulated annual precipitation (mm) and mean air temperature (°C) of the two future climate scenarios S2 and S4, from 2016 to 2050.

Table S1. Calibration and validation of the DAYCENT model 1–6 using the measured soil CO2 fluxes (g m−2 d−1) (the data in 2010–2012 for calibration and the data in 2014–2015 for validation), soil temperature (°C), soil moisture (cm3 cm−3), WFPS (%), switchgrass yield (Mg ha−1), and SOC (kg m−2 in the 0- to 10-cm depth) under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field.

Table S2. Calibration and validation of the DAYCENT model 7–12 using the measured soil N2O fluxes (g ha−1 d−1) (the data in 2010–2012 for calibration and the data in 2014–2015 for validation), soil temperature (soil-T, °C), soil moisture (soil-M, cm3 cm−3), WFPS (%), switchgrass yield (Mg ha−1), and NO3− (mg kg−1) under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field.

Table S3. DAYCENT predicted mean soil CO2 flux values from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4.

Table S4. DAYCENT predicted mean soil N2O flux values from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4.

Table S5. DAYCENT predicted mean switchgrass biomass yield from 2016 to 2050 under the high, medium, and low N rates at the shoulder and footslope positions in the switchgrass field based on the two future climate scenarios S2 and S4.