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# Sorghum biomass production in the continental United States and its potential impacts on soil organic carbon and nitrous oxide emissions

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## Abstract

National scale projections of bioenergy crop yields and their environmental impacts are essential to identify appropriate locations to place bioenergy crops and ensure sustainable land use strategies. In this study, we used the process-based Daily Century (DAYCENT) model with site-specific environmental data to simulate sorghum (*Sorghum bicolor* L. Moench) biomass yield, soil organic carbon (SOC) change, and nitrous oxide emissions across cultivated lands in the continental United States. The simulated rainfed dry biomass productivity ranged from 0.8 to 19.2 Mg ha<sup>-1</sup> year<sup>-1</sup>, with a spatiotemporal average of 9.7<sup>+2.1</sup><sub>-2.4</sub> Mg ha<sup>-1</sup> year<sup>-1</sup>, and a coefficient of variation of 35%. The average SOC sequestration and direct nitrous oxide emission rates were simulated as 0.79<sup>+0.38</sup><sub>-0.45</sub> Mg CO<sub>2</sub>e ha<sup>-1</sup> year<sup>-1</sup> and 0.38<sup>+0.04</sup><sub>-0.06</sub> Mg CO<sub>2</sub>e ha<sup>-1</sup> year<sup>-1</sup>, respectively. Compared to field-observed biomass yield data at multiple locations, model predictions of biomass productivity showed a root mean square error (RMSE) of 5.6 Mg ha<sup>-1</sup> year<sup>-1</sup>. In comparison to the multi State ( $n = 21$ ) NASS database, our results showed RMSE of 5.5 Mg ha<sup>-1</sup> year<sup>-1</sup>. Model projections of baseline SOC showed RMSE of 1.9 kg/m<sup>2</sup> in comparison to a recently available continental SOC stock dataset. The model-predicted N<sub>2</sub>O emissions are close to 1.25% of N input. Our results suggest 10.2 million ha of cultivated lands in the Southern and Lower Midwestern United States will produce >10 Mg ha<sup>-1</sup> year<sup>-1</sup> with net carbon sequestration under rainfed conditions. Cultivated lands in Upper Midwestern states including Iowa, Minnesota, Montana, Michigan, and North Dakota showed lower sorghum biomass productivity (average: 6.9 Mg ha<sup>-1</sup> year<sup>-1</sup>) with net sequestration (average: 0.13 Mg CO<sub>2</sub>e ha<sup>-1</sup> year<sup>-1</sup>). Our national-scale spatially explicit results are critical inputs for robust life cycle assessment of bioenergy production systems and land use-based climate change mitigation strategies.

## KEYWORDS

biomass, DAYCENT, emissions, sequestration, soil organic carbon, sorghum

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## 1 | INTRODUCTION

Bioenergy crops can help mitigate anthropogenic greenhouse gas (GHG) emissions as the carbon emitted during combustion of biofuels is balanced by the uptake from atmosphere through photosynthesis (Hughes, Lloyd, Huntingford, Finch, & Harding, 2010; Mishra, Torn, & Fingerman, 2013). Prior studies have estimated that biomass can be used to meet 15%–20% of the global predicted energy demand by 2050 (Beringer, Lucht, & Schaphoff, 2011), and about 25% by 2100 (Dale et al., 2014). The US Energy Independence and Security Act (EISA) of 2007 mandates an increase in the production of clean renewable fuels through the Renewable Fuel Standard, which requires 36 billion gallons of biofuels to be used in transportation fuel per year by 2022. Meeting the EISA goals requires substantial changes in land use patterns across the United States, which can impact the energy balance and biogeochemical cycles. Quantifying changes in soil organic carbon (SOC) and GHG emissions due to adoption of bioenergy crops at large spatial scales remain as grand challenges in conducting robust life cycle assessment of biofuels (McKone et al., 2011). National scale simulation of the bioenergy landscape using agroecosystem models capable of incorporating management practice and environmental effect can help (a) identify suitable locations to cultivate bioenergy crops; (v) assess soil- and site-specific environmental impacts of cultivating bioenergy crops at large spatial scales; and (c) reduce modeling uncertainties in downstream analysis such as life cycle assessments of biofuels and bioproducts.

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench] is a promising bioenergy crop because it is a drought-tolerant and high-yielding forage sorghum (Liu, Ren, Spiertz, Zhu, & Xie, 2015). Bioenergy sorghum maintains high biomass productivity under a wide range of environmental conditions and low inputs (Cui, Kavvada, Huntington, & Scown, 2018; Rooney, Blumenthal, Bean, & Mullet, 2007). Bioenergy sorghum can also be grown on marginal lands under constraints such as soil water deficits, soil salinity, and alkalinity without competing with food production (Dalla Marta et al., 2014; Regassa & Wortmann, 2014). High biological productivity, lower input requirements, and a wider range of adaptability to environmental conditions make sorghum an attractive feedstock option compared to other candidate annual bioenergy crops (Yu, XuZhang, & Tan, 2008).

Despite substantial research investments in developing sorghum as a bioenergy feedstock (e.g., the US Department of Energy ARPA-E TERRA program), little is known about the regional scale impact of sorghum cultivation on SOC change and nitrous oxide (N<sub>2</sub>O) emissions. Field studies focused on identifying the optimal nitrogen application and

crop residue removal rates to optimize the biomass yield and minimize soil GHG emissions. Storlien, Hons, Wight, and Heilman (2014) reported that nitrogen addition significantly increased N<sub>2</sub>O emissions, and incorporation of 50% sorghum crop residues to soil increased cumulative CO<sub>2</sub> emissions. The studies that focused on simulating sorghum biomass production using process models are limited to the field scale (Dou, Wight, Wilson, Storlien, & Hons, 2014; Wang et al., 2017), or used a coarse-scale land surface model that lacks a robust representation of the bioenergy crop and crop management conditions (Lee et al., 2018). More recently, a data-driven machine learning approach has been applied to predict the sorghum biomass productivity (Huntington, Cui, Mishra, & Scown, 2020). In this study, we quantify potential changes in SOC and N<sub>2</sub>O emissions due to cultivation of biomass sorghum across cultivated lands of continental United States using a process-based model. Our findings may help to identify suitable lands across continental United States to place bioenergy sorghum where economic biomass yield can be harvested with lower environmental impacts. Our results can also be used as input to life cycle assessments for biofuels to understand the net climate impacts of bioenergy production systems (McKone et al., 2011; Scown et al., 2012).

A wide range of process-based models are used to predict biogeochemical processes as a function of land management, soil properties, and climatic conditions to understand the SOC dynamics and GHG emissions from agricultural systems (Brilli et al., 2017; Coleman et al., 1997; Farina et al., 2011; Giltrap, Li, & Saggar, 2010). We used the Daily Century (DAYCENT) agroecosystem model (Del Grosso et al., 2001), which allows for a robust representation of diverse agricultural management practices while projecting biogeochemical changes both spatially and temporally. DAYCENT has been widely implemented to simulate the biomass yield, SOC changes, and GHG emissions from agricultural systems (Del Grosso et al., 2002, 2006, 2008). However, most of the DAYCENT model applications are limited to field scales due to the extensive data and computational power needed to run the model at large spatial scales. We applied the DAYCENT model over the continental United States at a 4 km grid resolution to understand the environmental impacts of cultivating bioenergy sorghum in the croplands and pasture and grass lands over the continental United States. The major objective of this study is to identify optimal locations in continental United States to cultivate sorghum with higher biomass yield and lower environmental impacts. The specific objectives of this study were to (a) predict the rainfed biomass productivity of sorghum on US cultivated lands; (b) quantify the potential changes in direct N<sub>2</sub>O emissions and SOC stocks due to sorghum adoption; and (c) identify the cultivated lands where sorghum adoption will provide economic

biomass yields and net carbon sequestration under rainfed conditions.

## 2 | MATERIALS AND METHODS

### 2.1 | DAYCENT model description

DAYCENT is a daily time step process-based agroecosystem model designed to simulate the biogeochemical cycles at a point scale (Del Grosso et al., 2001). DAYCENT is the extended daily version of the CENTURY model (Parton, Hartman, Ojima, & Schimel, 1998). It has the capability to simulate exchange of carbon and soil nutrients (nitrogen, phosphorus, and sulfur) between the atmosphere and terrestrial ecosystem, and other processes including soil water and soil temperature dynamics (Schimel et al., 2001). DAYCENT has been widely used to predict SOC change, GHG emissions, and plant productivity. Model inputs include climatic inputs; daily temperature and precipitation datasets, soil factors; texture, pH, hydraulic properties, and agricultural management; historic details on land use; and fertilizer, tillage, and other management activities. The DAYCENT model simulates decomposition and nutrient mineralization of plant litter and soil organic matter. The crop submodule in DAYCENT simulates plant growth and phenology, net primary productivity and its allocation to different compartments (grain, root, and shoots), and the C:N ratio of these plant compartments. The growing degree-day approach is used for management scheduling. This approach enables scheduling agricultural management as a function of surface air temperature, known as the heat unit approach. The heat unit for the plant is determined in the model based on long-term climate data and the crop-specific base temperature.

### 2.2 | Study area, weather, and soil input

We included three land cover types (croplands, pastures, and grasslands; hereafter “cultivated” lands) based on the National Land Cover Database (Yang et al., 2018) that could be converted to bioenergy crop production in the continental United States. The model simulation was conducted at a 4 km grid scale and limited to areas where the land cover type in each grid is more than 50% cropland, grassland, and/or pasture (Figure S1). The 30 year (1989–2018) daily precipitation and minimum and maximum air temperature data were extracted from the Global Historical Climatology Network (GHCN) datasets of National Centers for Environment Information and used for weather input to the model (Menne, Durre, Vose, Gleason, & Houston, 2012). There are over 4,161 weather stations with 30 year datasets

across the continental United States. The average annual daily temperature and average annual precipitation during 1989–2018 are presented in Figure S2. The weather generator-simulated weather data based on 30 year historic data were used for the long-term historic simulation of the native vegetation. For assigning the weather station data to each grid, the nearest weather station based on haversine distance from the centroid of the grid was used. The major soil parameters for the model include the multilayer soil texture, bulk density, soil moisture characteristics curve data, hydraulic conductivity, soil organic matter, and soil pH. The Soil Survey Geographic (SSURGO) database was used to build the model input database, and calculations were made for the soil water characteristics curve data (wilting point and field capacity) using the pedotransfer function (Saxton & Rawls, 2006; Soil Survey Staff, 2015). A summary of the data types and the sources used in this study is presented in Table S1.

### 2.3 | Regional simulation, land use, and DAYCENT model setup

The study area was divided into 4 km grid cells, and the simulations were conducted at the centroid of the grid cell. The DAYCENT model is designed to explicitly run at a point scale with no horizontal connections among the cells. Considering the number of available GHCN weather stations and computational efficiency for processing the daily timescale regional input/output of the model, this study was conducted at a 4 km grid, which is common across the environmental modeling community for regional scale applications (Daly et al., 2000; Oubeidillah, Kao, Ashfaq, Naz, & Tootle, 2014). The DAYCENT model was run for 4,000 years to achieve the steady-state values for soil carbon and nitrogen pools to reflect the natural conditions of land prior to start of agriculture (Basso et al., 2011). Region-specific grass types were used for the equilibrium run based on the data used in the US Environmental Protection Agency Inventory of US GHG emissions and sinks (USEPA, 2015). Land use and management history for the past and present were compiled from different data sources. Historical management from initial tillage to the modern agricultural period was simulated with crop rotation and a management scheme compiled at the Major Land Resource Area level from different historical data sources (Ogle et al., 2010). Modern day agriculture management representation was based on the multiyear National Land Cover Database analysis. The historical database was used to represent the average annual nitrogen fertilizer rates for each of the agricultural crops (USEPA, 2005). Bioenergy sorghum was cultivated in 2008 to study the impact of decade-long cultivation of the bioenergy crop. The assumptions for

large-scale cultivation of sorghum included (a) use of heat unit-based agricultural management; (b) the same cultivar of sorghum across the study area; (c) rainfed conditions; (d) common fertilizer application rate of 120 kg N/ha; and (e) an aboveground biomass removal rate of 90%. Sorghum is commonly grown in Southern region of United States, as a result, agricultural management data across continental United States were not available. The fertilizer rate that we applied was based on the recommendation for economic yield of sorghum for southern region, and this rate will not limit the crop growth in other regions of United States (Contreras-Govea, Lauriault, Marsalis, Angadi, & Puppala, 2009; Cotton, Burow, Acosta-Martinez, & Moore-Kucera, 2013; Han et al., 2012). We used uniform agricultural management and model parameters across the study region to understand the variability in sorghum biomass productivity across region as a function of land use history, weather, and soil properties.

The model setup was automated using an R script (R Core Team, 2018), which enabled reading the weather data from the GHCN database and generating weather files, reading the data from the SSURGO database and generating the soil data files and updating the site-specific and crop parameters for each grid cell across the study area. The results are presented as the spatial mean with prediction range due to interannual climate variability and soil properties represented as the first and the third quartile.

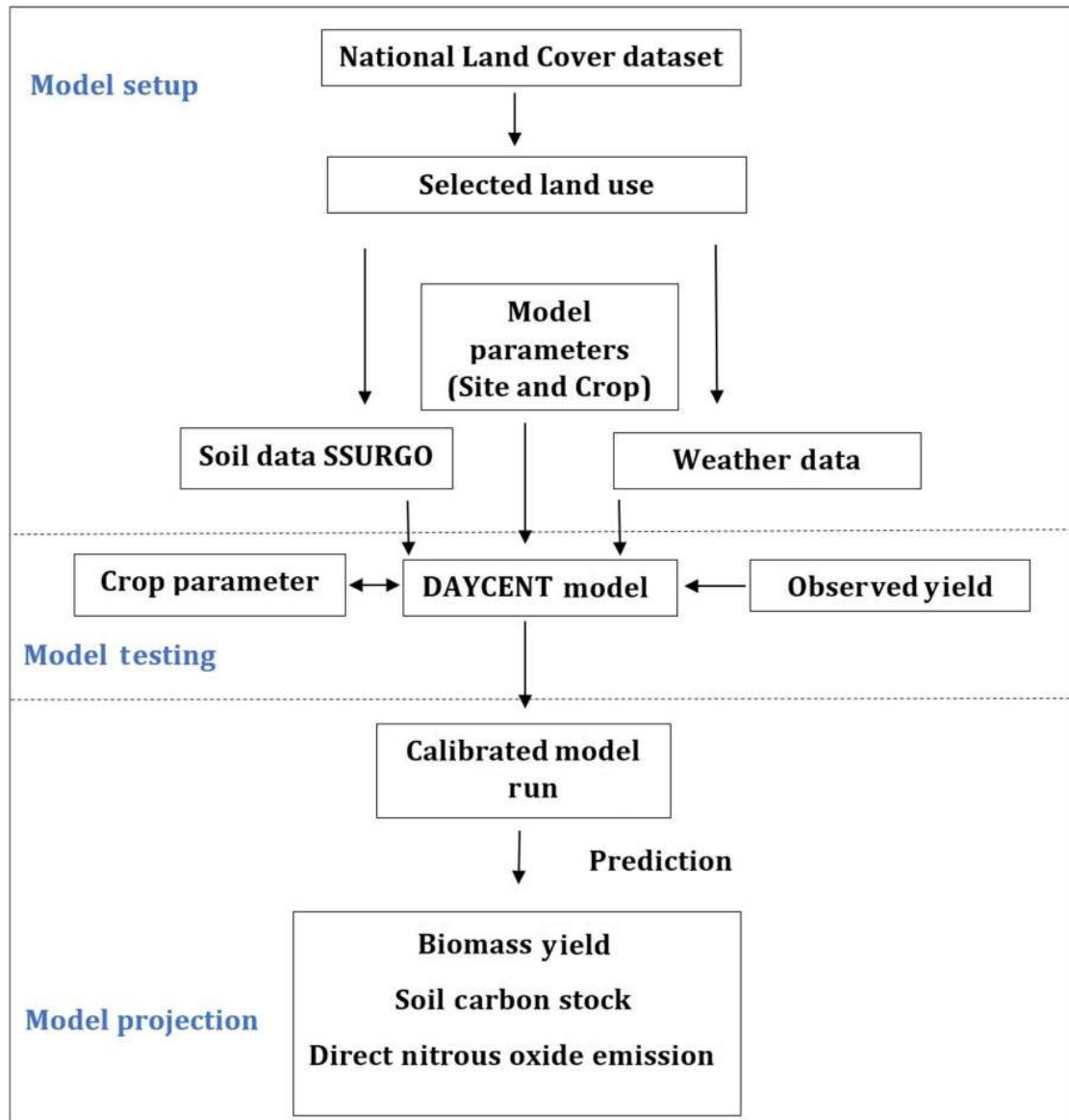
## 2.4 | Model calibration and parameterization

Model calibration for bioenergy sorghum has been conducted in an earlier study for simulating field-scale measurement of water content, SOC, and soil temperature (Wang et al., 2017). In our study, the crop parameters were changed to represent the field-scale sorghum biomass yield for the multiple locations. Manual calibration was preferred over autocalibration, as DAYCENT parameter sensitivity and ranges were well understood based on previous studies of sorghum (Duval et al., 2013; Duval, Ghimire, Hartman, & Marsalis, 2018; Wang et al., 2017). We attempted to represent the variability in sorghum yield due to change in environmental factors (soil properties, temperature, precipitation, and solar radiation) across the study domain. The observed yield from a 5 year study (2008–2012) under multiple rainfed locations with standard agronomic practices was used for the model calibration (Gill et al., 2014). Our DAYCENT predictions were validated using sorghum yield values from the literature (Chaganti et al., 2020; Wang et al., 2017; Wight et al., 2012). The geographic distribution of the validation sites represents major rainfed sorghum growing regions in the continental United States.

Furthermore, the predicted biomass yield was compared with the time series multi State sorghum biomass yield data from the National Agricultural Statistics Services (NASS) survey dataset (NASS, 2018). Model performance was evaluated using root-mean-square error (RMSE). RMSE is a square root of the average of squared differences between the observation and model prediction values.

The baseline SOC prediction of the DAYCENT model was compared with observed SOC data points ( $n = 654$ ) across continental United States using Rapid Carbon Assessment database (West, Wills, & Loecke, 2013). Due to a lack of experimental data on trace gas fluxes on fields growing bioenergy sorghum, we validated our  $N_2O$  emission predictions based on the biomass productivity and SOC. This approach has been well documented to provide reliable validation of gas fluxes (Adler, Grosso, & Parton, 2007; Del Grosso et al., 2002, 2006; Duval et al., 2013). After calibration, the model was updated with a calibrated set of parameters and simulation was executed in the nine-node, 324-core cluster computing system at Argonne's Laboratory Computing Resource Center in the parallel environment. Parallel execution was implemented in R (<https://www.r-project.org/>) using the parallel package. The schematic for implementation of the entire modeling steps is presented in Figure 1.

The objective function of the model parameterization was to reduce the RMSE of the sorghum dry biomass prediction across the calibration sites to find representative sets of parameter combination. A list of the model parameters with default values and selected values is provided in Table S2. The model parameters which control the crop production due to solar radiation and the water stress multipliers were the two most sensitive parameters regulating the biomass yield (Table S2). The crop-specific energy-biomass conversion factor (PRDX (1)) represents the genetic potential of the crop, PRDX (1) was adjusted to 3.0 to represent the higher yield potential of bioenergy sorghum (Table S2). The crop-specific energy-biomass conversion factor was a sensitive parameter for biomass yield prediction. Other parameters (PPDF (1) and PPDF (2)) relating to the curve defining temperature were also found to be sensitive to biomass yield. The parameter to represent the water stress coefficient on potential growth was decreased to 0.2 to fit the water stress curve for sorghum to the relationship described in the FAO Irrigation and Drainage paper no. 56 (Allen, Pereira, Raes, & Smith, 1998). Zhang, Hansen, Trout, Nielsen, and Paustian (2018) demonstrated that the crop-specific water stress coefficients in the FAO 56 method can be used for deriving the DAYCENT parameters. This parameter resulted in the yield difference between the eastern and western regions of the United States where rainfall patterns are different, regulating the biomass yield.



**FIGURE 1** Schematic showing steps included for large-scale application of Daily Century (DAYCENT) model

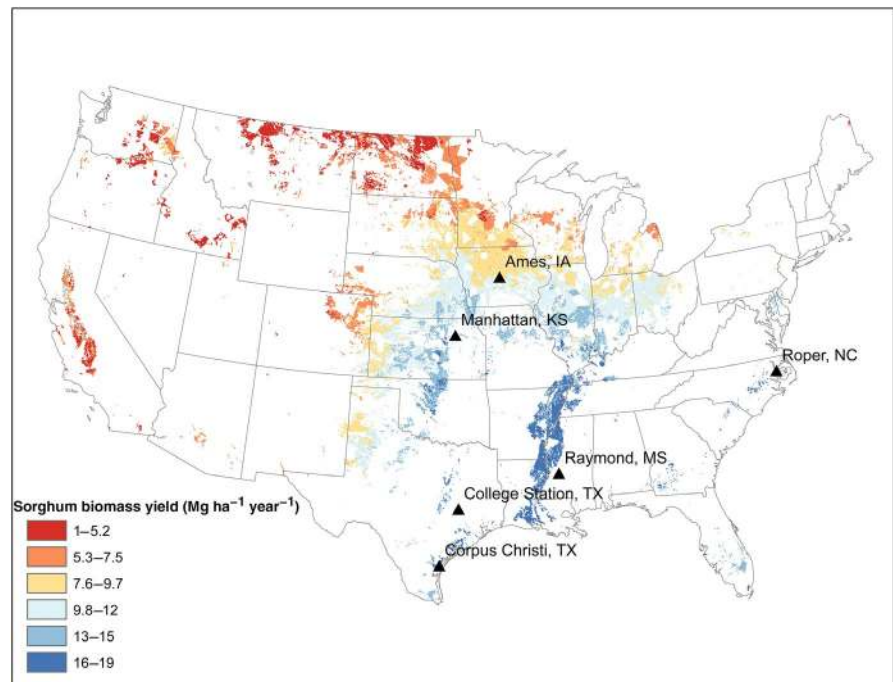
### 3 | RESULTS

#### 3.1 | Biomass yield prediction

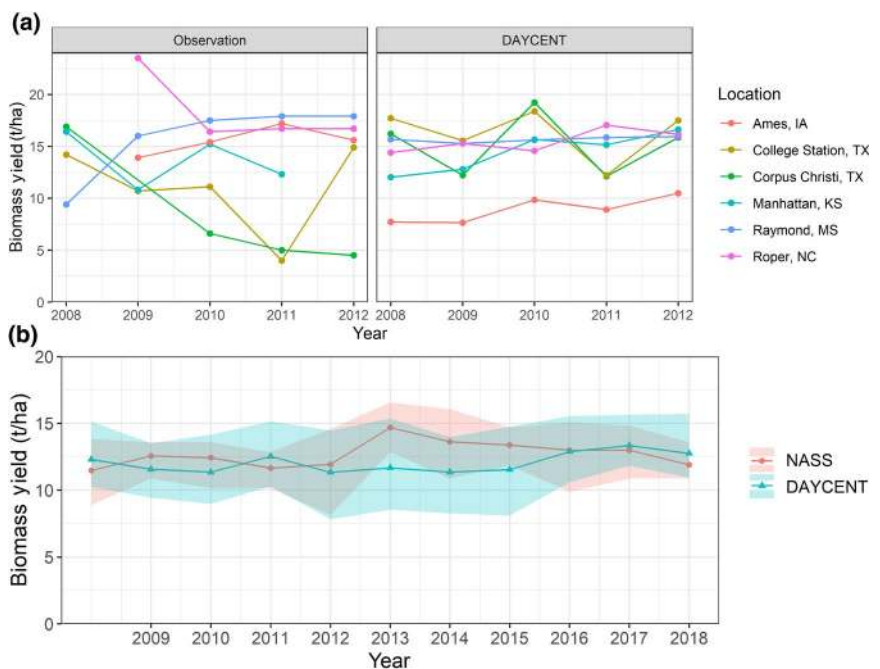
The simulated rainfed dry biomass yield (hereafter referred to as biomass) values for continental United States ranged from 0.8 to 19.2 Mg ha<sup>-1</sup> year<sup>-1</sup>, with a spatiotemporal average of 9.7<sup>+2.1</sup><sub>-2.4</sub> Mg ha<sup>-1</sup> year<sup>-1</sup> and a coefficient of variation of 35% (Figure 2). The positive and negative values in the upper- and lowercases represent uncertainty ranges based on an interquartile range of predictions. The range of simulated yields, including first (Q1) and third quartile (Q3) of the yield map based on 10 year simulations, is presented in Figure S3. The spatial variations in the projected yields are attributed to the environmental conditions of the study area. The yield response was primarily governed by

precipitation and temperature (Figure S2). Cultivated lands in the Southern United States and Kansas have higher daily average annual temperature and precipitation, and thus are projected to have higher average sorghum biomass yield (12.5<sup>+2.0</sup><sub>-2.3</sub> Mg ha<sup>-1</sup> year<sup>-1</sup>). The comparison of simulated and observed biomass yield across multiple years is presented in Figure 3a. The model was able to represent year-to-year variability in yield and multiyear average yield for each of the six locations. The RMSE value for the projected biomass yield for the selected year is 5.6 Mg ha<sup>-1</sup> year<sup>-1</sup>. Model predictions are close to observed yields in the validation data for the average yearly yield across all locations. In 2009, the average yearly predicted yield across all locations was 13.1 compared to observed yield of 15 Mg ha<sup>-1</sup> year<sup>-1</sup> (Figure 3a). For individual locations, the average yearly yield is well aligned to the validation data for all locations

**FIGURE 2** Rainfed biomass yield of sorghum across the continental United States simulated using the Daily Century model; locations of the Regional Feedstock Partnership Partnership Trails (black triangles) used for validation



**FIGURE 3** Comparison of the Daily Century (DAYCENT) model sorghum biomass yield with (a) multilocation bioenergy field trail (Gill et al., 2014) and (b) multi State ( $n = 21$ ) National Agricultural Statistics Services (NASS) Sorghum yield datasets (NASS, 2018)



except Corpus Christi, Texas. In Corpus Christi, the model over-predicted biomass yield compared to the observed yield; however, the model was able to simulate the year with a higher biomass yield (Figure 3a). The model was unable to predict the wide range of observed variability in biomass yield for Texas. The model underpredicted the yield for Ames, IA. The model prediction closely represented the observed multiyear yield trend in biomass for all other four locations (Figure 3a). The time series comparison of DAYCENT yield with NASS dataset shows close year-to-year match in ensemble mean and range of predictions with

RMSE of  $5.5 \text{ Mg ha}^{-1} \text{ year}^{-1}$  (Figure 3b). The comparison statistics of the NASS yield and DAYCENT prediction are presented in Table S3.

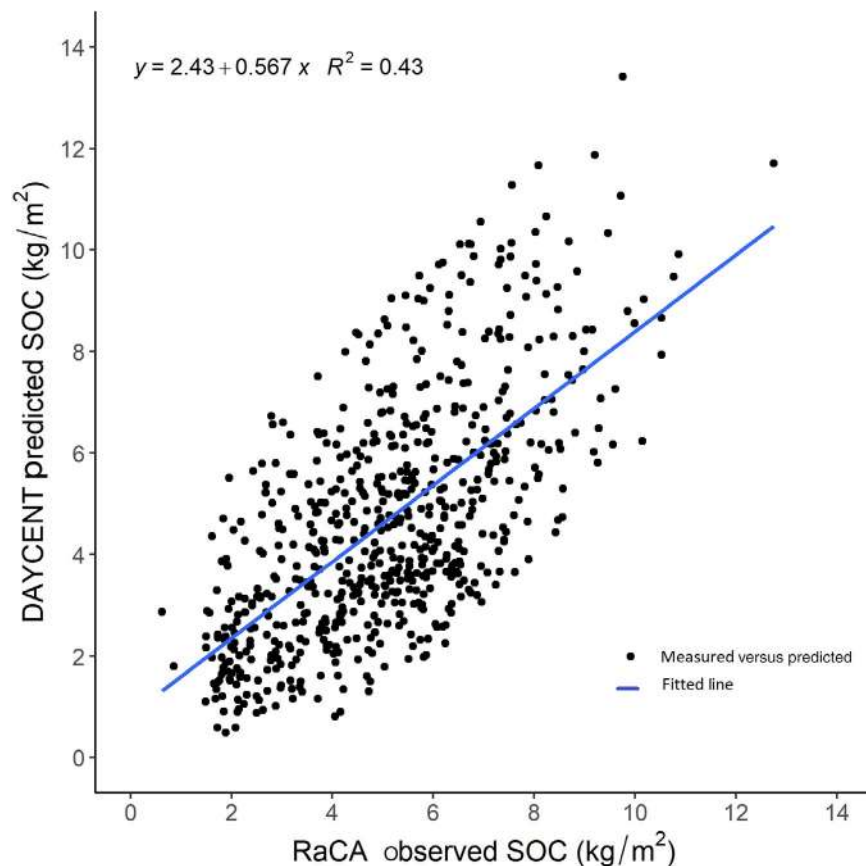
### 3.2 | Soil organic carbon change, direct nitrous oxide emissions, and hotspot analysis

The DAYCENT model was set up to simulate the SOC dynamics for the topsoil (0.2 m). The baseline SOC prediction of DAYCENT model showed  $r^2$  of .43 and RMSE of  $1.9 \text{ kg/}$

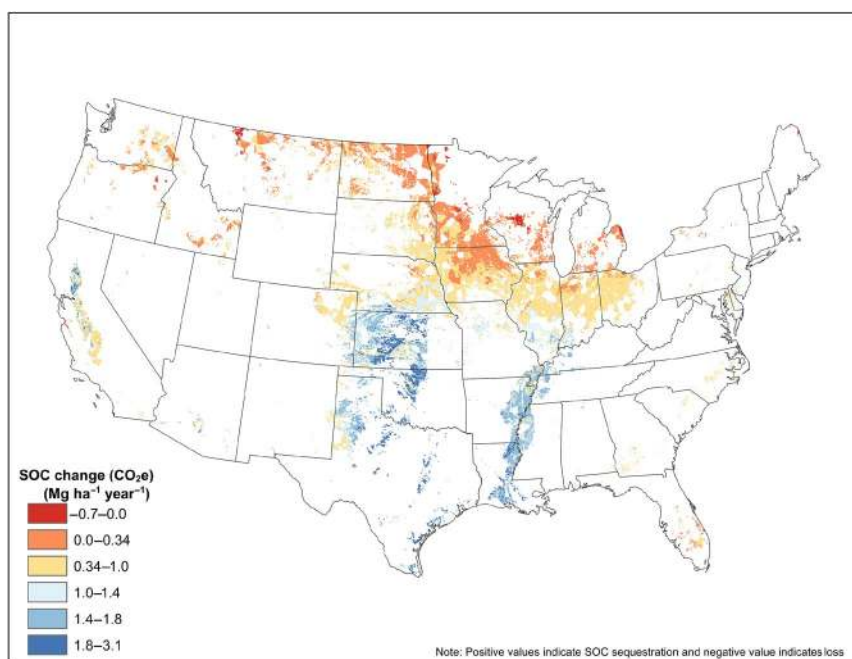
$\text{m}^2$  when compared with 654 observed point across continental United States (Figure 4).

Simulated SOC change for the continental United States ranged from  $-0.76$  to  $3.0 \text{ Mg CO}_2\text{e ha}^{-1} \text{ year}^{-1}$  with a spatial mean of  $0.79^{+0.38}_{-0.45} \text{ Mg CO}_2\text{e ha}^{-1} \text{ year}^{-1}$  for decade-long sorghum cultivation (Figure 5). The spatial mean SOC

sequestration for the Southern region plus Kansas was  $1.54^{+0.33}_{-0.27} \text{ Mg CO}_2\text{e ha}^{-1} \text{ year}^{-1}$ . A few states in the Upper Midwest showed net soil carbon emissions resulting from long-term sorghum cultivation (Table S4). The SOC map before and after decade-long cultivation of bioenergy sorghum is presented in Figure S4. The spatiotemporal average



**FIGURE 4** Comparison of Daily Century (DAYCENT) predicted baseline soil organic carbon (SOC) stocks with Rapid Carbon Assessment (RaCA) SOC database (West et al., 2013) across continental United States



**FIGURE 5** Simulated mean soil organic carbon stock change for topsoil (0.2 m) due to decade-long (2009–2018) sorghum cultivation across the continental United States

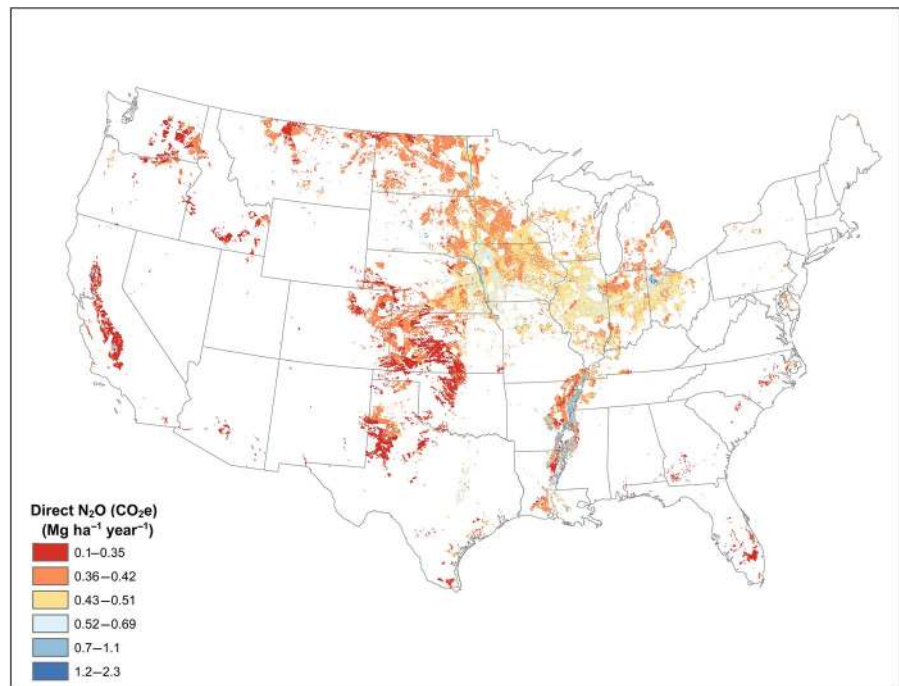


direct N<sub>2</sub>O emission due to sorghum cultivation was simulated as  $0.38^{+0.04}_{-0.06}$  Mg CO<sub>2</sub>e ha<sup>-1</sup> (Figure 6). The range of direct N<sub>2</sub>O emissions including the first (Q1) and third quartile (Q3) of the emission map based on decade-long simulations is presented in Figure S5. Higher N<sub>2</sub>O emissions are simulated in the states of Arkansas, Louisiana, Mississippi, and Missouri (Table S4). Simulated direct N<sub>2</sub>O emissions are lower for the Western states, intermediate for Midwestern states, and highest for the Southeastern states. We also compared N<sub>2</sub>O emission values with bulk density data from the data basin project (<https://databasin.org/maps/>)

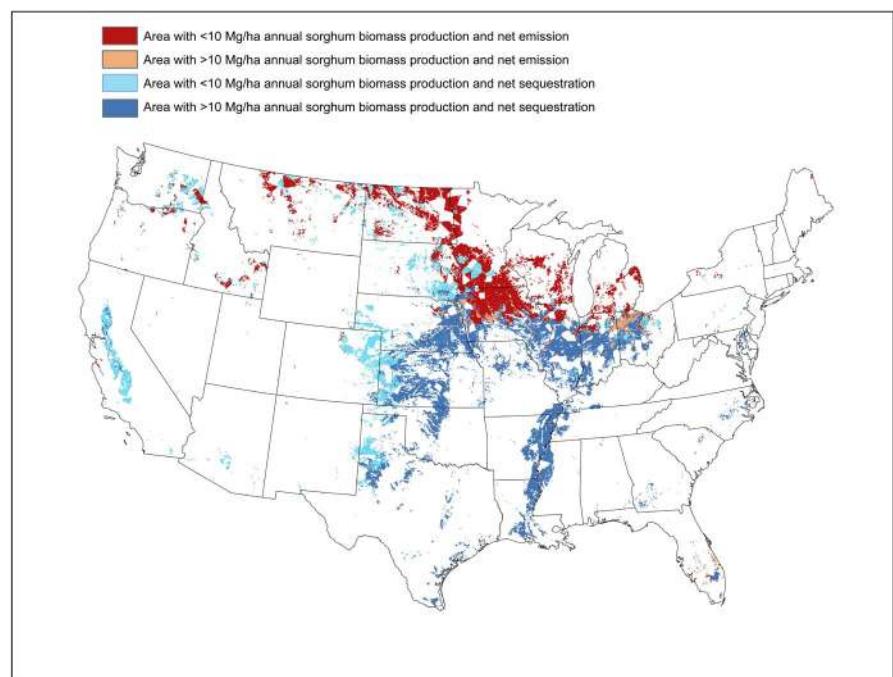
which uses the National Resources Conservation Service soil water holding capacity and soil texture data to predict the soil bulk density. The croplands with a bulk density range of 1.29–1.36 g/cm<sup>3</sup> showed more N<sub>2</sub>O emissions. Lower N<sub>2</sub>O emissions were predicted in the areas where bulk density ranged from 1.37 to 1.55 g/cm<sup>3</sup>.

Results based on overlay of productivity and emission maps showed that the states including Lower Midwest and Southern US states can produce more than 10 Mg/ha dry rainfed biomass with net carbon sequestration (Figure 7). The area with economic biomass yield had simulated biomass

**FIGURE 6** Simulated mean emission of direct nitrous oxide as carbon dioxide equivalent during decade-long (2009–2018) sorghum cultivation across the continental United States



**FIGURE 7** Cultivated lands of the continental United States that will produce different sorghum biomass yields with net carbon sequestration and emission; different classification criteria are defined in the legend



yield and net carbon sequestration of  $11.9^{+2.3}_{-1.9}$  Mg ha<sup>-1</sup> year<sup>-1</sup> and  $1.2^{+0.4}_{-0.4}$  Mg CO<sub>2</sub>e ha<sup>-1</sup> year<sup>-1</sup>, respectively. The Upper Midwest states showed less than 10 Mg/ha biomass yield with net carbon emission, and Western states showed lower biomass yield with net carbon sequestration (Figure 7). Our results suggest that 10.2 million ha of cultivated lands of the Southern and Lower Midwestern states will produce sorghum biomass yield >10 Mg/ha with net carbon sequestration. The spatial average biomass yield, SOC change, and N<sub>2</sub>O emissions of all the simulated states are presented in Table S4.

## 4 | DISCUSSION

We generated spatially explicit estimates of potential biomass sorghum productivity, SOC change, and N<sub>2</sub>O emissions across cultivated lands of the United States. The point scale process model was scaled up using detailed environmental, soil, and management representations to identify suitable locations for production of biomass sorghum across the continental United States. Our national-scale results are critical inputs to life cycle assessments, which require full GHG accounting and form the basis of important biofuel policies including the Low Carbon Fuel Standard and Renewable Fuel Standard. Yield predictions are also crucial for techno-economic analyses, as the tonnage-normalized cost of farming inputs and average transportation from the field to the biorefinery are all dependent on feedstock yields.

Sorghum biomass yield is sensitive to crop parameters relating to the radiation use efficiency, temperature, water stress, and carbon-to-nitrogen ratio. Our findings are consistent with the findings of earlier studies (Dou et al., 2014; Field, Marx, Easter, Adler, & Paustian, 2016; Necpálová et al., 2015; Stehfest, Heistermann, Priess, Ojima, & Alcamo, 2007; Wang et al., 2017). Earlier studies predicted sorghum biomass yields ranging from 1 to 25 Mg ha<sup>-1</sup> year<sup>-1</sup>, with higher yields in the Southeastern United States. Our predicted average sorghum biomass yield and its spatial distribution are consistent with the observations/predictions of (Dou et al., 2014; Lee et al., 2018). Lower yield predictions in the Western United States are due to water-limiting conditions (Lee et al., 2012). The yield variability is higher in sorghum, and our predictions also represent those yield variabilities. The county-level data show a 69% coefficient of variation in rainfed sorghum yield (Kukul & Irmak, 2018); our results predict a 35% coefficient of variation in predicted biomass yield. The greater variability in sorghum biomass yield in the drier regions under rainfed conditions is due to variability in soil moisture availability for crop growth, which is very common in the Western United States (Gill et al., 2014). The model simulates crop production based on incoming photosynthetic radiation and the radiation use efficiency of a crop, where water stress based on available

water and potential evapotranspiration represents biomass yield decline. In this study, parameters for higher genetic potential dominated the yield response in the Southern region with optimum temperature, precipitation, and solar radiation. Biomass productivity in the Upper Midwestern United States was lower due to lower temperature and shorter growing seasons. The optimum temperature requirement for the vegetative growth and development of sorghum ranges from 26 to 34°C (Maiti, 1996). A previous experimental study documented a decrease in growth rate of sorghum under lower temperature treatments (Lyons, 2012). An earlier study has also documented the sensitivity of sorghum to chilling temperature, making sorghum cultivation challenging in higher latitude (Ercoli, Mariotti, Masoni, & Arduini, 2004). Chilling significantly affects plant growth in early spring, resulting in reductions in sorghum biomass yields. The yields in the Southeastern states are higher and correlated to higher temperature and precipitation in the region (Lee et al., 2018; Regassa & Wortmann, 2014). Lower biomass yield in the croplands of Western states is due to a lack of sufficient precipitation to support optimal crop growth. The model representation for high-yielding varieties and the yield response to extreme weather events need to be further improved to better represent new advancements in the genetic engineering. The average yield of  $12.5^{+2.0}_{-2.3}$  Mg ha<sup>-1</sup> year<sup>-1</sup> in the Southern states can produce ethanol yields up to around 2,856–3,920 L ha<sup>-1</sup> year<sup>-1</sup> (Tang, Li, Li, & Xie, 2018).

The spatial pattern of the SOC stock predicted from our study across cultivated lands in the continental United States represents the general observed spatial pattern of SOC in the agricultural region of the United States (Tifafi, Guenet, & Hatté, 2018). SOC increased after decade-long cultivation of sorghum in most of study locations except in very few locations at higher latitudes. Bioenergy sorghum favors SOC sequestration due to higher root biomass (15%–20% of total biomass) resulting in increased annual input of organic matter to soil (Olson et al., 2012). Carbon flux from soils is sensitive to variability in temperature and precipitation (Lucht et al., 2002; Poulter et al., 2014; Schwalm et al., 2012). Temperature and precipitation are the major drivers governing yield response which defines the carbon sequestration.

Our predicted mean N<sub>2</sub>O emission over continental United States is close to 1.25% of N input, which is consistent with IPCC recommendations (IPCC, 2006). In addition, our model projection shows variation in N<sub>2</sub>O emission across study region due to variation in soil texture. Direct N<sub>2</sub>O is produced from the nitrogen cycle due to denitrification and nitrification of the organic nitrogen. DAYCENT simulates the nitrification process based on soil ammonium concentration, volumetric soil water content, relative saturation, soil temperature, soil pH, and soil bulk density. The denitrification process is simulated based on the soil

nitrate concentration, labile C, O<sub>2</sub>, and soil texture. Soil moisture is the major driver of N<sub>2</sub>O emissions, as it defines the availability of oxygen in soil (Butterbach-Bahl, Baggs, Dannenmann, Kiese, & Zechmeister-Boltenstern, 2013). In the croplands with high moisture (more than 60% of water-filled pore space), the end product of denitrification is N<sub>2</sub> gas (Bouwman, 1998). Our predictions of N<sub>2</sub>O emissions are also correlated with the soil bulk density. The bulk density can also be related to the soil moisture, and studies have used bulk density to predict soil moisture (Vereecken, Maes, Feyen, & Darius, 1989). In other words, the croplands with fine-textured soil resulted in higher N<sub>2</sub>O emissions in comparison to croplands with coarse textured soil. Our findings of the soil texture dependence of N<sub>2</sub>O emissions are consistent with findings of earlier studies which also reported higher N<sub>2</sub>O emission from fine-textured soil compared to coarse-textured soil (Gaillard, Duval, Osterholz, & Kucharik, 2016). Del Grosso et al. (2006) reported 2%–2.5% N<sub>2</sub>O emissions for fine-textured clay soil in comparison to 0.8%–1% for coarse-textured sand soil. DAYCENT model assumes higher SOC in fine-textured soil slows decomposition of plant residue compared to coarse texture soil. The higher SOC provides the C for denitrifying microbes leading to increased N<sub>2</sub>O emission (Bouwman, Boumans, & Batjes, 2002).

Our study comes with some limitations and assumptions. Sorghum is dominantly grown in Southern United States as a result, there is lack of data on agricultural management for sorghum over continental United States. We used a constant fertilizer application rate of 120 kg N/ha based on the recommendation for the economic yield of dryland sorghum cultivation (Ogunlela, 1988; Restelatto, Pavinato, Sartor, Einsfeld, & Baldicera, 2015). Other limitations of this study include the use of constant phenotype and parameter representation over space and time.

In summary, our study made reasonable predictions of the average annual biomass sorghum yield across cultivated lands of the continental United States. The spatial average of simulated biomass sorghum yield for the continental United States was  $9.7^{+2.1}_{-2.4}$  Mg ha<sup>-1</sup> year<sup>-1</sup>. The spatial average of simulated biomass sorghum production for locations with economic productivity and net carbon sequestration was  $11.9^{+2.3}_{-1.9}$  Mg ha<sup>-1</sup> year<sup>-1</sup>. The productivity of biomass sorghum was found to be sensitive to temperature and precipitation; sorghum yield was lower in the upper latitude due to the sensitivity of sorghum to chilling temperature. The cultivated lands of Southern and Lower Midwest states with higher daily average annual temperature and precipitation are projected to have higher sorghum biomass yield. Our results of SOC sequestration showed the suitability of Southern states for sorghum cultivation with a net carbon sequestration of  $1.54^{+0.33}_{-0.27}$  Mg CO<sub>2</sub>e ha<sup>-1</sup> year<sup>-1</sup>. Our

result predicts higher N<sub>2</sub>O emissions for the locations with fine-texture soils. Based on the biomass yield and the emission trends of N<sub>2</sub>O, the Southern states excluding the locations with fine-textured soils are ideal places for cultivating sorghum. Midwestern states including Kansas, Missouri, and Illinois predicted sorghum yield benefits with lower N<sub>2</sub>O emissions. Overall, our results indicate that an area of 10.2 million ha of cultivated lands of the Southern and Lower Midwestern states can sustain economic biomass sorghum yield with net carbon sequestration under rain-fed conditions. Future studies on biomass sorghum productivity and its environmental impacts should focus on region-specific sorghum genotype and crop management representations.

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## DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available in the Supporting Information of this article. Additional data and code can be obtained from the corresponding author upon reasonable request.

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## SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section.

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