Empirical Approach to Estimate Net Ecosystem Exchange Using High Frequency Mesonet Observations across Potential Switchgrass Establishment Landscapes in Oklahoma

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Abstract

Monitoring net ecosystem carbon dioxide (CO2) exchange (NEE) using eddy covariance (EC) flux towers is quite common, but the measurements are valid at the scale of tower footprints. Alternative ways to quantify and extrapolate EC-measured NEE across potential production areas have not been explored in detail. To address this need, we used NEE measurements from a switchgrass (Panicum virgatum L.) ecosystem and detailed meteorological measurements from the Oklahoma Mesonet and developed empirical relationships for quantifying seasonal (April to October) NEE across potential switchgrass establishment landscapes in Oklahoma, USA. We identified ensemble area for potential switchgrass expansion regions and created thematic maps of switchgrass productivity using geostatistics and GIS routines. The purpose of this study was not to calibrate the model for estimating NEE in the future but to explore if model parametrizations based on high temporal frequency meteorological forcing can be used to construct reliable estimates of NEE for evaluating the source-sink status of organic carbon. Based on EC measurements, empirical models, a) rectangular hyperbolic light-response curve and b) temperature response functions, were fitted to estimate gross primary production (GPP) and ecosystem respiration (ER) on a seasonal scale. Model performance validated by comparing EC-measured seasonal NEE for three years showed good-to-strong agreement ($0.29 < R2 < 0.91$; $p < 0.05$). Additionally, total seasonal NEE estimates were validated with measured biomass data in three additional locations. The estimated seasonal average net ecosystem production (NEP =-NEE) was 3.97 ± 1.92 (S.D.) Mg C ha-1. However, results based on a simple linear model suggested significant differences in NEP between contrasting climatic years. Overall, the results from this study indicate that this new scaling-up exercise involving high temporal resolution meteorological data may be a helpful tool for assessing spatiotemporal heterogeneity of switchgrass production and the potential of switchgrass fields to sequester carbon in the Southern Great Plains of the United States.

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Monitoring net ecosystem carbon dioxide (CO_2) exchange (NEE) using eddy covariance (EC) flux towers is quite common, but the measurements are valid at the scale of tower footprints. Alternative ways to quantify and extrapolate EC-measured NEE across potential production areas have not been explored in detail. To address this need, we used NEE measurements from a switchgrass (*Panicum virgatum* L.) ecosystem and detailed meteorological measurements from the Oklahoma Mesonet and developed empirical relationships for quantifying seasonal (April to October) NEE across potential switchgrass establishment landscapes in Oklahoma, USA. We identified ensemble area for potential switchgrass expansion regions and created thematic maps of switchgrass productivity using geostatistics and GIS routines. The purpose of this study was not to calibrate the model for estimating NEE in the future but to explore if model parametrizations based on high temporal frequency meteorological forcing can be used to construct reliable estimates of NEE for evaluating the source-sink status of organic carbon. Based on EC measurements, empirical models, a) rectangular hyperbolic light-response curve and b) temperature response functions, were fitted to estimate gross primary production (GPP) and ecosystem respiration (ER) on a seasonal scale. Model performance validated by comparing EC-measured seasonal NEE for three years showed good-to-strong agreement ($0.29 < R^2 < 0.91$; $p < 0.05$). Additionally, total seasonal NEE estimates were validated with measured biomass data in three additional locations. The estimated seasonal average net ecosystem production (NEP =-NEE) was 3.97 ± 1.92 (S.D.) Mg C ha^{-1}. However, results based on a simple linear model suggested significant differences in NEP between contrasting climatic years. Overall, the results from this study indicate that this new scaling-up exercise involving high temporal resolution meteorological data may be a helpful tool for assessing spatiotemporal heterogeneity of switchgrass production and the potential of switchgrass fields to sequester carbon in the Southern Great Plains of the United States.

1 Introduction

Fossil fuel combustion has been identified as a primary carbon dioxide (CO_2) emission source and a key factor in the mounting human-induced climate crises. The development of carbon-neutral or carbon-negative alternative fuel is an urgent global priority to curtail the increasing consumption of fossil fuel and mitigate the threats of the climate crisis. Various cellulosic biofuel species are proposed as a cornerstone of a low-carbon economy with the potential to displace or reduce petroleum consumption for transportation (Robertson *et al.*, 2017). Unfortunately, legislative initiatives on biofuel production have expanded grain-based ethanol production and garnered negative attention due to risks associated with nitrous oxide emissions, nitrate pollution, soil carbon loss (Gelfand *et al.*, 2013), and food security (Demirer *et al.*, 2012). Instead, opting for perennial exemplary biomass crops such as switchgrass (*Panicum virgatum* L.), miscanthus (*Miscanthus* × *giganteus*), and hybrid poplar trees (*Populus spp.*) would be a better choice for future energy portfolios because of their substantial energy return on investment (Ohlrogge *et al.*, 2009).

Various policies and incentives (e.g., the European Union's Renewable Energy Directive (2018/2001) and the U.S. Energy Independence and Security Act, 2007) are in place currently to encourage biofuel production and development. Relatedly, the enactment of the Biomass Crop Assistance Program (BCAP) in 2008 was aimed to incentivize biomass for bioenergy production. To achieve energy independence from foreign oil, the U.S. Energy Independence and Security Act, 2007, has mandated the production of 16 billion gallons (1 gallon = 3.785 liters) of cellulosic ethanol by 2022. The most recent 2016 Billion-Ton Report from the U.S. Department of Energy has identified willow (*Salix spp.*), miscanthus, and switchgrass as perennial feedstocks with the potential for profitable production (Langholtz, 2016).

Switchgrass is a productive, perennial C_4 grass native to the tallgrass prairie regions of the U.S. and one of the promising model energy crops for bioenergy feedstock (Wright, 2007). It is a dual-purpose forage and biofuel feedstock, which requires minimal management. It is effective at storing soil organic carbon, even below depths greater than 30 cm, due to its prolific and deeper root systems (Lee *et al.*, 2007, Liebig *et al.*, 2005). Switchgrass has larger potential for greenhouse gas sinks compared to cultivated croplands (Adler *et al.*, 2007). Ecologically, switchgrass is dominant in the central Great Plains region and renders various ecosystem services, that include but are not limited to, livestock forage, nitrate-nitrogen leaching mitigation (Brandes *et al.*, 2017, Griffiths *et al.*, 2021), provision for wildlife habitat (Marshall *et al.*, 2017), phytoremediation (Guo *et al.*, 2019, Shrestha *et al.*, 2019), and wind and water erosion protection (Liebig *et al.*, 2005). Long-term data have demonstrated the feasibility of switchgrass for liquid fuel production across a broad geographic region of the U.S. (Mitchell *et al.*, 2014).

As the Agriculture Improvement Act of 2018 has reauthorized the extension of the Conservation Reserve Program, production of switchgrass is likely to occur in the marginally productive land, minimizing the competition with other field crops (Bigelow *et al.*, 2020). The Great Plains of the U.S. has the potential to become a pivotal location for lignocellulosic feedstock production (Martinez-Feria & Basso, 2020). Although the feasibility of switchgrass for biofuel production has been demonstrated for the U.S. (Mitchell *et al.*, 2014), the existing scientific literature is not yet rich enough to provide information on switchgrass productivity and its carbon sink potential across large geographical and temporal scales (Behrman *et al.*, 2013). Lately, there has been a growing interest in studying carbon dynamics in switchgrass to understand its potential to offset anthropogenic greenhouse gases and make switchgrass a promising bioenergy crop (Eichelmann *et al.*, 2016, Kasanke *et al.*, 2020, Slessarev *et al.*, 2020). Various approaches have been utilized to predict switchgrass productivity, such as the use of Robel pole for ocular estimates (Schmer *et al.*, 2010), process-based plant growth models (Behrman *et al.*, 2013, Brown *et al.*, 2000, Hartman *et al.*, 2011, Kiniry *et al.*, 1996, McLaughlin *et al.*, 2006), empirical modeling (Jager *et al.*, 2010), and remote and proximal sensing (Foster *et al.*, 2016, Gu *et al.*, 2015). Although remote sensing is a proven tool to provide spatially comprehensive ecosystem activity (Churkina *et al.*, 2005), satellite-based information is not readily available at finer temporal and spatial resolutions. Moreover, remote sensing observations will not be available now for potential future production areas.

Information on ecosystem-level study of switchgrass productivity and its carbon dynamics in the Southern Great Plain regions of the U.S. is lacking. Only a few studies have reported carbon dynamics of switchgrass ecosystems for few years only based on EC measurements (Eichelmann *et al.*, 2016, Liebig *et al.*, 2005, Skinner & Adler, 2010, Wagle & Kakani, 2014b, Wagle & Kakani, 2014c, Wagle *et al.*, 2015). The EC flux towers continuously measure ecosystem-level net exchange of CO_2, H_2O, energy, and other trace gases between the land surface and the atmosphere. However, EC systems provide measurements for their footprint areas or fetch lengths, which usually ranges from 100 m to few kilometers depending on several factors, including EC tower height, wind speed, and vegetation properties (Gockede *et al.*, 2004). Additionally, direct measurements of fluxes using EC towers are cost-prohibitive and limited to flat topography with uniform vegetation only (Baldocchi, 2008, Baldocchi, 2003). Thus, these site-level measurements need to be extrapolated or upscaled at larger spatial scales to estimate the regional carbon balance (Wofsy et al.,19993) and facilitate carbon cycling research (Gilmanov *et al.*, 2005). In this paper, we developed empirical models to derive switchgrass productivity during the growing season (April through October) using EC-measured NEE from a switchgrass ecosystem and easily accessible time series meteorological data from the Oklahoma Mesonet and validated the estimates of NEE to four different sites using ancillary measures (e.g., NEE, biomass). Additionally, we characterize seamless switchgrass productivity estimates for the potential switchgrass production areas in Oklahoma. This proposed method can be implemented elsewhere for a regional prediction of switchgrass or any other bioenergy production potential species.

2 Materials and Methods

2.1 Net ecosystem CO_2 exchange measurements

Eddy covariance measurements, equipped with a CSAT3 sonic anemometer (Campbell Scientific Inc., Logan, UT, U.S.) and LI-7500 open-path infrared gas analyzer (IRGA, LI-COR Inc., Lincoln, NE, U.S.), were taken in a switchgrass (cv. Alamo) field located at Oklahoma State University South Central Research Station, Chickasha, Oklahoma (35° 2' 24'' N, 97° 57' 0'' W, 330 m above sea level) after the first year of its establishment (2010). The EC data recorded at 10 Hz frequency were processed using *EddyPro* software (LI-COR Inc., Lincoln, NE, U.S.) to compute 30-min eddy fluxes. Data quality was assessed by the degree of energy balance closure [latent heat (LE) + sensible heat (H)]/ [net radiation (Rn) – soil heat flux (G)]. Energy balance closures of 0.77 and 0.83 were reported for 2011 and 2012, respectively (Wagle and Kakani, 2014d), which were within the typical range for EC experiments (Foken, 2008). The study area was under abnormally dry to exceptional drought during the study period. Details on eddy flux measurements and data processing have been extensively described previously (Wagle and Kakani, 2014c; a; Wagle et al., 2014; Wagle et al., 2015).

2.2 Site description

The State of Oklahoma was chosen as a study region given the presence of one of the foremost mesoscale-level weather monitoring networks (Oklahoma Mesonet, http://mesonet.org/) that records research-quality grade weather data. According to the Köppen-Geiger climate classification, Oklahoma's climate has distinct zonation, with a humid subtropical climate in the east to a semi-arid climate in the west (Kottek et al., 2006). The state covers the region bounded by 94° 29' 08.90" W–103° 00' 06.631" W longitude and 33° 38' 17.7" N–37° 00' 00.473" N latitude. Topographic elevation in Oklahoma ranges from 87 m near Little River to 1518 m above mean sea level on Black Mesa. A distinct north-south temperature gradient and east-west precipitation gradient are present. The average annual temperature is around 14°C along the northern border and 16.6 °C at the southern border (see, http://climate.ok.gov/index.php/site/page/climate_of_oklahoma). Average annual precipitation ranges from 432 mm in the far western panhandle to 1422 mm in the far southeast. The state encompasses twelve level III eco-regions and forty-six level IV eco-regions (Woods et al., 2005). Oklahoma has 14 million hectares of cropland area distributed throughout nine agricultural districts (USDA, 2017a) (Northeast, Southeast, East Central, South Central, Central, North Central, Southwest, West Central, and Panhandle). Forty-nine percent of the total cropland area is grass/ pasture, followed by 18% deciduous forest, and 11% wheat-grown areas. As per the recent Conservation Reserve Program statistics (USDA, 2017b), 277,349 ha of land in Oklahoma are enrolled in Conservation Reserve Program (https://bit.ly/3Ftlu1j, accessed May 23, 2021). This suggests there is an abundance of land for biomass feedstock production and a potential large market for biofuels in Oklahoma.

The soil type at the flux tower siting was McClain silt loam (fine, mixed, super active, thermic, Pachic Argiustolls) (Foster et al., 2015). The site where flux tower is located received a total of 525 and 673 mm precipitation during 2011 and 2012 compared to 30-year average (1981–2010) rainfall of 896 mm. The aboveground switchgrass (cultivar Alamo) biomass data was manually harvested at the end of the growing season (late September through early October) from Stillwater Agronomy Research Station, Stillwater, Oklahoma (36°07'03.7"N 97°05'37.0"W); Wes Watkins Agricultural Research and Extension Center, Lane, Oklahoma(34°18'17.9"N 96°00'12.3"W); South Central Research Station, Chickasha, Oklahoma (35°02'38.9"N 97°54'50.2"W); and Southern Great Plains Research Station, Woodward, Oklahoma (36°25'18.2"N 99°24'17.6"W) from 2011 to 2014. These stations represent various ecoregions of Oklahoma (Tables

Table 1), and their mean monthly temperature and average monthly total precipitation are shown in Fig. 1.

2.3 Procuring and processing the Mesonet data

Five-minute interval weather data for 110 environmental monitoring stations across Oklahoma (Fig. 2) were acquired from the Oklahoma Mesonet (Mesoscale network) from 2011 to 2014. The automated weather stations collect statewide weather data, with a minimum of one site in each of Oklahoma's seventy-seven counties to ensure spatial meteorological differences across landscapes are captured well (Brock et al., 1995; McPherson et al., 2007). Most of the aboveground Mesonet measurements are averaged over five minutes from measurements sampled every three seconds, except for the barometer and the event driven rain gauge. Data included relative humidity (RH, %), air temperature at 1.5 m (T_{air}, °C), solar radiation (*Srad*, Wm^{-2}), liquid precipitation (Rain, mm), and soil temperature under native vegetation at 5 cm (TS05, °C). Instruments used to measure these variables are summarized in (Table 2). Data was checked thoroughly for missing and erroneous observations and processed to calculate maximum, minimum, and average values for every 30-minutes.

2.4 Deriving coefficients for NEE estimates

Empirical equations were developed based on EC measurements during the 2011 and 2012 growing seasons in a switchgrass field (8 ha) at the South-Central Research Station, Chickasha, Oklahoma. Light-saturated NEE (NEE_{sat}) was calculated as a function of air temperature (temperature ≥ 5.9 ºC and PPFD ≥ 50 μ mol $m^{-2}s^{-1}$). Daytime respiration (DR) was calculated using a quadratic function of air temperature, whereas nighttime respiration (NR) was calculated using an exponential function of soil temperature. Temperature response curves were developed for NEE_{sat}, apparent quantum efficiency (α), DR, and NR. Based on these values, 30-minute NEE values were generated as a function of NEE_{sat}, photosynthetic photon flux density (PPFD), and α. We applied the same equations from April through October to the rest of the entire study period and locations.

The sign convention of NEE used in this study is that CO_2 uptake by the ecosystem is negative, whereas CO_2 release to the atmosphere is positive. The study window (i.e., growing season) was limited to the April 1-October 31 period for each year. We estimated values of PPFD (μmol m^{-2} s^{-1} of photons with wavelengths of 0.4-0.7 μm) using solar radiance values. In this study, a conversion factor of 1.892 was used to convert downwelling global solar radiation into photosynthetically active radiation (PAR) (Varlet-Grancher et al., 1981). The methodology evolves according to the following equations:

$$PAR = 0.48 \times SI \quad (1)$$

$$PPFD = 4.6 \times PAR \quad (2)$$

Following Tetens (1930), the saturation vapor pressure (e_s) (kPa) at a given air temperature, T (°C) was computed as:

$$es = 0.6108 exp \frac{17.27 \times T}{T + 237.3} \quad (3)$$

We calculated the saturation vapor pressure (e_s) at maximum (T_{max}) and minimum air temperature (T_{min}) by replacing T with T_{max} and T_{min} in the above equation.

$$e_s = 0.5[e^0(T_{max}) + e^0(T_{min})] \quad (4)$$

Where $e^0(T_{max})$ and $e^0(T_{min})$ are the saturated vapor pressure at maximum and minimum temperature, respectively. The following equation recommended by Allen et al. (1998) was used to calculate actual vapor pressure (e_a) [kPa].

$$e_a = \frac{e^0(T_{min}) \times \frac{RH_{max}}{100} + e^0(T_{max}) \times \frac{RH_{min}}{100}}{2} \quad (5)$$

Vapor pressure deficit (VPD) was calculated as a difference between saturation vapor pressure and actual vapor pressure.

Ecosystem respiration (ER) is the sum of autotrophic and heterotrophic respiration. Accurate quantification of ER is imperative for understanding switchgrass carbon dynamics as respiration emits a substantial proportion of daytime photosynthetic assimilates to the atmosphere. Measurement of CO_2 flux during nighttime by the EC system is underestimated due to weak mixing in less turbulence and presence of deep boundary layer; leading to systematic and methodological error (Wofsy et al., 1993; Ruimy et al., 1995; Lavigne et al., 1997). ER values were determined using the exponential temperature function developed by Lloyd and Taylor (1994) as:

$$ER = R_0 e^{(\beta T_s)} \quad (6)$$

where R_0 (μmol CO_2 m^{-2} s^{-1}) is the base respiration at Ts = 0 °C, β (°C^{-1}) is a constant related to temperature sensitivity coefficient (Q_{10}). The exponential model based on T_s explained 60% of the seasonal ER variation for the site when volumetric soil water content was > 0.2 m^3 m^{-3} [ER = 0.72 × *exp (*0.08 × T_s), $P < 0.0001$] (Wagle & Kakani, 2014a). Daily ER was also modeled as proposed by Reichstein et al. (2003) using daily average values of nighttime soil temperature and soil moisture as the main drivers of the nonlinear regression function.

$$ER = R_{ref}\, exp(a + b \times RSWC) \left(\frac{1}{T_{ref} - T_0}\right) \left(\frac{RSWC}{RSWC_{\frac{1}{2}} + RSWXC}\right) \quad (7)$$

In this equation, R_{ref} (μmol m^{-2} s^{-1}) is the ecosystem respiration under standard conditions (at T_{ref} = 21°C; non-limiting water), T_{ref} (°C) is the reference temperature, T_0 (°C) is the lower temperature limit for the ER which was fixed at -46 °C as in the original model of Lloyd and Taylor (1994), and RSWC is the soil water content. $RSWC_{1/2}$ is the fraction of soil water content where half-maximal respiration occurs. This exponential temperature-respiration function could explain more than 50% of seasonal ER variation at soil moisture > 0.20 m^3 m^{-3}. We applied equation 8 to calculate ER throughout the growing season using soil temperature measurements as average of soil temperature records collected at 5 cm and 10 cm depths under the sod. Finally NEE data were partitioned into GPP and ER using the rectangular hyperbolic light-response function developed by Falge et al. (2001).

$$NEE = \frac{\alpha \times GPP_{max}}{\alpha \times PPFD + GPP_{max} + ER} \quad (8)$$

where α is the apparent quantum yield, PPFD is photosynthetic photon flux density (μmol m^{-2} s^{-1}), GP_{max} is the maximum canopy CO_2 uptake rate (μmol m^{-2} s^{-1}) at light saturation, and ER is respiration rate at zero PPFD. Limitation of higher VPD on photosynthesis was observed (Wagle and Kakani, 2014d) as Eq (7) failed to provide good fits for the NEE values. This problem was addressed by calculating GPP_{max} as the exponential decreasing function at high VPD, as suggested by Lasslop et al. (2010). A modification of the hyperbolic light response curve was imposed to account for the VPD limitation of GPP by replacing GPP_{max} with GP_0.

$$GPP0\, exp\big(-k(VPD - VPD_0)\big)_{0_{max}} \quad (9)$$

$$GPP0_{0_{max}} \quad (10)$$

where VPD_0 threshold was set to 1 kPa as in Lasslop et al. (2010). Additionally, *k* parameter was estimated using nonlinear least squared regression in SAS software (SAS Institute Inc., 2013, Cary, NC, U.S.). The NEE at light saturation (NEE_{sat}), contingent upon average temperature and PPFD values, was derived using the equations 11-13.

$$If T_{avg} > 5.9, NEE_{sat} = \left(\left(31.7659 - 0.8456 \times T_{avg} - 32.8766\right) - 2.006 \times T_{avg-32.8766}\right); else 0 \tag{11}$$

$$If PPFD < 50,0, else NEE_{sat} \tag{12}$$

Light saturated NEE limited by VPD was computed as follows:

$$NEE_{sat,VPD} = NEE_{sat} \times exp\left(-0.2026 \times (VPD - 1)\right) \tag{13}$$

In addition, ER values were generated using the following equation:

$$If PPFD \leq 50, ER = -0.7205 \times exp(0.0814 \times TS_{05}); \quad else, ER = \left(-0.5135 \times T_{avg} + 0.115 \times T_{avg}\right)^2 \tag{14}$$

Afterward, we computed α as following:

$$\alpha = \left(0.0035 \times T_{avg}\left(0.00008 \times T_{avg}{}^2\right)\right) \tag{15}$$

Finally, the NEE values were calculated as following:

$$If NEE_{sat,VPD} = 0, NEE_{final} = ER; \quad else, NEE_{final} = \frac{(NEE_{sat,VPD}) \times \alpha \times PPFD}{(NEE_{sat,VPD}) + PPFD + \alpha} \tag{16}$$

Total NEE (g CO_2 m^{-2}) was computed using the following conversion factor:

$$\frac{\sum NEE \times 1800}{22.6 \times 1000} \tag{17}$$

Gaps in the data were filled using average values immediately before and after the gap. We calculated cumulative amounts of seasonal NEE that was sequestered per unit area.

2.5 Identifying potential switchgrass establishment areas in Oklahoma

According to the Conservation Reserve Program (CRP) - USDA Farm Service statistics of 2014, up to 20% of the county area was under the CRP program in Oklahoma (Fig 3a). Especially, the counties in western Oklahoma and Oklahoma Panhandle area (Texas, Cimarron, Beaver, Harper, Ellis, and Grant) had most of the land area dedicated to the CRP. We aggregated six subclasses: switchgrass, fallow, pasture, shrubland, and grassland as defined in the 2008-2014 USDA-NASS Cropland Data Layer (CDL) to identify potential switchgrass production areas in Oklahoma. The raster data were imported into ArcGIS and reclassified to show only potential switchgrass production areas (Fig 3b).

As mentioned earlier, seasonal average NEE values were calculated for each of the Mesonet sites. Calculated seasonal NEE values were then interpolated using ordinary kriging interpolation (Dhakal et al., 2020). The mask identified for potential switchgrass production area was applied to the annual NEE surface to generate seasonal switchgrass NEE across the state.

2.6 Calibration and Validation

We used three years (2011-2013) of EC measurements of CO_2 fluxes, the first two years of data for developing the empirical equations, and the third year of data to validate the predictions made by our empirical models. Conceptually, NEE can be linked to total biomass production. Hence, we used end-of-season aboveground switchgrass biomass data as well to validate the NEE estimates with measured aboveground switchgrass biomass from 2011 to 2013 in four locations (Lane, Stillwater, Chickasha, and Woodward) in Oklahoma. Linear regression was used to compare paired measurements of half-hourly EC-based NEE and half-hourly NEE estimates. To quantify the accuracy of prediction, root mean square error (RMSE) was also reported, along with the coefficient of determination and slope.

$$\text{RMSE} = \sqrt{\sum_{i=1}^{n} \frac{(P_{i} - O_{i})}{N}} \qquad (19)$$

$$R^2 = \left(\frac{n(\sum XY) - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}\right)^2 \qquad (20)$$

3 Results

Pairwise comparisons of estimated NEE at half-hourly, monthly, and seasonal scales were made with the measured NEE. For each year, we observed good agreements between the half-hourly measured NEE and the estimated NEE, with R^2 values ($p < 0.05$) of 0.59, 0.63, and 0.63; and RMSE values of 4.78, 4.51, and 4.36 μ mol CO_2 m^{-2} s^{-1}, for 2011, 2012, and 2013 respectively (Fig. 4a). The agreement was similar for 2012 and 2013, with R^2 values of 0.63 and slope of ~0.5. For all the years, the slope of the regression line was less than one, suggesting underestimates of NEE values.

For each month of the growing season, there was a good agreement between the measured and estimated half-hourly NEE values (R^2 values ranged between 0.52 and 0.74) (Fig. 4b). The agreement was highest for May (R^2 = 0.74, slope =0.46, p<0.05) and lowest for October (0.52, slope

= 1.74, $p < 0.05$). Further, we aggregated monthly NEE values for each year and compared them against the aggregated measured NEE values. A strong agreement between the monthly cumulative measured and estimated NEE was observed for 2013, which was a wetter year ($R^2 = 0.91$, $p < 0.05$) followed by a drier year 2012 ($R^2 = 0.81$, $p < 0.05$). However, the agreement was poor between the measured and estimated monthly cumulative NEE values for 2011, which was a severe drought year ($R^2 = 0.29$, $p < 0.05$). Contrarily, the slope of the regression line was closer to 1.0 for 2011 than 2012 and 2013. Looking at the sink-source status of the switchgrass ecosystem monthly, we observed that the switchgrass ecosystem was a small source of CO_2 for July and August of 2011 and sink for the rest of the months in the growing season but sink for CO_2 for the entire growing season of 2012 and 2013. Based on the estimated NEE values, May, and June (peak growth periods) had the highest estimated NEE (negative sign convention) among the studied months across all three years. However, a more accurate and complete NEE measurement and estimates of the true source-sink status of the switchgrass ecosystem establishment warrants year-round, long-term studies.

Further, we computed seasonal NEE during 2011-2014 for Oklahoma State University's four different research stations located at Stillwater, Lane, Chickasha, and Woodward (for site description, refer to Table 1) using five-minute interval weather data for the Oklahoma Mesonet stations in proximity to the research stations (STIL, LANE, CHIC, and WOOD) as mentioned earlier. For these locations, we compared the seasonal NEE estimates with the end-of-the-season aboveground switchgrass biomass collected from 2011 to 2014. Results showed strong agreements between the measured aboveground switchgrass biomass and the seasonal carbon uptake by the switchgrass ecosystem in all four stations ($R^2 > 0.93$, $p < 0.05$) (Fig. 6).

Upon observing a good agreement between seasonal NEE estimates and switchgrass aboveground biomass production, we computed the NEE estimates for all active Oklahoma Mesonet stations. The distribution of the seasonal NEE for each year is shown in Fig. 7. We generated seasonal C uptake grids for the potential switchgrass production sites across the state of Oklahoma from 2011 to 2014 (Fig. 8). We used the ordinary kriging interpolation method to generate seasonal NEE raster surface for those years. The year 2011 was a severe drought year and reported as the second driest year in Oklahoma since 1925 (Shivers and Andrews, 2013). Statewide seasonal NEE for 2011 was recorded as the lowest among the four (278.5 ± 154 g C m^{-2}). The effect of drought is visible in the annually interpolated NEE surface (Fig. 8). The year 2014 had the highest seasonal NEE estimates (493 ± 181 g C m^{-2}).

For all the sites across 2011–2014, the average seasonal switchgrass NEE was estimated at around 1870 ± 703 g CO_2 m^{-2} (5.1 Mg CO_2 ha^{-1}). NEE values ranged from -468 g CO_2 m^{-2} to -4093 g CO_2 m^{-2} for the Mesonet sites at Tipton, Oklahoma and Clayton, Oklahoma, respectively. The Mesonet site at Tipton had temperature data missing for eight days, which resulted in the NEE estimates to be the lowest among all the Mesonet sites.

4 Discussion

The concept for estimating carbon uptake per absorbed PAR has been demonstrated previously (Monteith, 1972; Sinclair and Horie, 1989; Goetz and Prince, 1999). Based on the radiation use efficiency concept, various models have been developed to simulate carbon exchange between the atmosphere and terrestrial biosphere that account for spatiotemporal dynamics in the ecosystem for both potential and natural vegetation (Kirschbaum et al., 2001; Fisher et al., 2014). In addition, use of regression models have been also used to quantify the ecosystem CO2 exchange. Zhang et al. (2011) used piecewise regression model that included normalized difference vegetation index (NDVI), phenological metrics, weather data, and soil water holding capacity to show that grasslands in the U.S. Great Plains are net C sink (0.3 to 47.7 g C m^{-2} yr^{-1}). Moreover, the ecological literature contains a plethora of peer-reviewed scientific data highlighting the use of remotely and proximately sensed vegetation production measurements and eddy flux measurements to estimate and upscale NEE to a regional level (Emmerton et al., 2016; Reitz et al., 2021). For example, Asrar et al. (1984) demonstrated that cumulative NDVI measurements through the growing season may be used to obtain estimates of GPP. Because the coarse spatial resolution of the satellite derived measurements has been identified as a source of error, coupling Landsat TM and Landsat ETM+ with flux tower measurements using image fusion and regression tree approach was found to be effective for regional NEE estimations (Fu et al., 2014). With improvement in high-resolution satellite sensors, shorter satellite revisit time, high frequency weather data, and advanced data processing and machine learning algorithms, remote sensing approach can be more appealing in regions with limited in-situ observation networks (Sharma and Dhakal, 2021).

Recently, Liu et al. (2021) used various environmental variables (net radiation, soil water content, soil temperature, precipitation, vapor pressure deficit, and wind speed) to predict NEE for 10 different biomes. The authors used trained XGBoost and Random Forest model to >10 years of Fluxnet sites measurement across a wide range of biomes and obtained accurate prediction of NEE for forest, savanna, and grassland ecosystems ($0.55 > R^2 < 0.81$) (Liu et al., 2021). Our approach also relies completely on deriving relationships between the environmental variables such as air temperature, soil temperature, and solar radiation to compute half-hourly NEE estimates. The Oklahoma Mesonet records meteorological data at high temporal frequency (5-min intervals), offering a unique possibility to produce empirical estimates of regional NEE of switchgrass when extrapolated using measured NEE. Estimates of mean NEE across the Mesonet sites ranged from 2.78 ± 1.54 Mg C ha^{-1} in 2011 to 4.93 ± 1.81 Mg C ha^{-1} in 2014. The NEE estimates from the semiarid sites of Oklahoma are similar to the EC flux measurements of NEE measured in a switchgrass ecosystem in Central Illinois. (4.53 ± 0.2 Mg C ha^{-1}) (Zeri et al., 2011). Furthermore, the NEE measurements acquired from a mature switchgrass stand in Southwestern Ontario for the year 2014 was 3.36 ± 0.38 Mg C ha^{-1}.

The temporal behaviour of NEE in the switchgrass ecosystem demonstrated seasonal and day-to-day variations. Additionally, the sptatiotemporal simulations illustrate the effect of microclimate variability on the carbon balances is captured well for carbon budget related studies in switchgrass ecosystem on a regional scale. This indicates that our approach using fine temporal resolution meteorological forcings can capture and describe a range of variation of biophysical factors in switchgrass ecosystems. Improvement in NEE estimates can be achieved by calibrating and validating with site-specific flux and meteorological measurements.

Further inclusion of belowground biomass would significantly improve NEE estimates results at localities. To our knowledge, there is no other empirical method that is robust across the interest of scale of time and space, which simulates the switchgrass carbon uptake. In this study, the NEE measured by EC technique at a location was extrapolated to quantify carbon sequestration potential across potential switchgrass areas in Oklahoma using 30-minute averaged Mesonet data. As it has been highlighted in the literature, upscaling of EC-based carbon fluxes to large regions has been conducted using different approaches such as data-driven (empirical, statistical models) or data assimilation approaches (ecosystem models, parameter estimation techniques) (Xiao et al., 2012). Empirical estimates of net primary productivity for terrestrial plant communities were computed from climatology-derived actual evapotranspiration (Rosenzweig, 1968). Gross primary production (GPP) in the terrestrial ecosystems of the southern U.S. was estimated by scaling up leaf assimilation rates of the shaded and sunlit canopy and factoring it with the daytime length (Tian et al., 2010). Likewise, GPP modelling for boreal and temperate forest ecosystems was based on light use efficiency, daily mean temperature, vapor pressure deficit (VPD), and soil water content (Makela et al., 2008). In their study of carbon fluxes in ponderosa pine forest (*Arctostaphylos patula* and *Purshia tridentata*), Law et al. (2001) also reported that Biome-BGC process model simulated carbon budgets have been found to underestimate NEE compared to EC measurements.

Since our study was only limited to the growing season, source/sink dynamics for the entire year were not captured. However, it is imperative to understand the responses of NEE to various climatic conditions such as pluvial, drought, and normal years. Uncertainties in this study arise from parameterizing the model with limited site and simplification of some of the ecosystem processes that may not truly capture the exact variability of real phenomena. Most of the coefficients and constants were generated from our calibration site. These values may vary spatially; therefore, additional studies are necessary to investigate and reduce the uncertainty in the model's applicability. We only conducted validation of NEE at the local level. Since this study was performed for potential switchgrass growing areas, ground truth data for all the sites are not available. If the switchgrass growing areas are large enough to be captured with satellite imagery, large-scale validation can be performed using high-resolution remotely sensed data. There is also a potential for benefiting from usage of current technology such as Uncrewed Aerial Vehicles (UAVs), which can capture the data on-demand on a custom scale. However, that is beyond the scope of this study. Future studies should focus on improving this empirical approach to include year-round estimates of NEE under various climatic conditions.

5 Conclusions

The seasonal carbon balance of a switchgrass ecosystem was evaluated using an estimate of net ecosystem CO_2 exchange (NEE). The models use radiation use efficiency approach, with air temperature, soil temperature, vapor pressure deficit, and quantum use efficiency as modifying factors. Empirical equations for estimating NEE of CO_2 in a switchgrass ecosystem were generated and validated against eddy covariance tower measured NEE along with field data for switchgrass biomass production and high frequency (5-min intervals) meteorological data from four locations. Our results illustrate the importance of carbon balance model development on a temporal and spatial scale. This approach can be used to compare direct carbon flux measurements or when flux measurements data are unavailable for a better understanding of source-sink status of the switchgrass ecosystems. The study could be helpful in adjusting cropping systems and management practices for bioenergy production and understanding of carbon sequestration at a regional level. Undoubtedly, with improved datasets at a range of scales and computing power, we will enhance our ability to predict and capture spatial patterns of carbon exchange in switchgrass landscapes. However, we also acknowledge the fact that such extrapolations should be done with care because of accompanying uncertainties which require a thorough understanding of the subject matter. Given the findings here, we recommend pursuing spatial modeling of NEE over a large spatial domain with additional field measurements representative of that agroecological domain.

6 Author Contributions

KD, VGK, and PW: conceptualization. KD and VGK: formal analysis. VGK: fund acquisition. KD and SS: original draft writing, data analysis, and visualization. KD, VGK, and PW: revision and editing. All authors contributed to the article and approved the submitted version.

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Tables

Table 1. Characteristics of the switchgrass grown fields, including soils (USDA, 2017), the United States Environmental Protection Agency (EPA) ecoregion (Level IV ecoregion of are shown in parenthesis), and the United States Department of Agriculture Plant Hardiness Zone.

Site	**Soil name**	**Dominant taxonomic classification**	**EPA Ecoregion**	**USDA Plant Hardiness Zone**
Lane	Bernow	Fine-loamy, siliceous, active, thermic Glossic Paleudalfs	South Central Plains (35d)	7b
Stillwater	Easpur	Fine-loamy, mixed, superactive, thermic Fluventic Haplustolls	Central Great Plains (27o)	7a
Chickasha	Dale McLain	a) Fine-silty, mixed, superactive, thermic Pachic Haplustolls b) Fine, mixed, superactive, thermic Pachic Argiustolls	Central Great Plains (27d)	7 7a
Woodward	a) Devol b) Eda	a) Coarse-loamy, mixed, superactive, thermic Typic Haplustalfs b) Mixed, thermic Lamellic Ustipsaments	Central Great Plains (27q)	6b

Table 2 Summary of the sensors used in the Oklahoma Mesonet network.

Variable	**Sensor**	**Unit**	**Accuracy**
Air Temperature at 1.5 m	Thermometrics Air Temperature	°C	± 0.5 °C
Rainfall	Met One Tipping-Bucket	mm	±5% over the range of 0 to 5 cm hr^{-1}
Soil Temperature, under sod (5 cm)	Stainless steel encased 10K thermistor probe, thermocouple sensor	°C	±0.5 °C
Solar Radiation	LI-200S Pyranometer	$W\ m^{-2}$	±5%

Figures

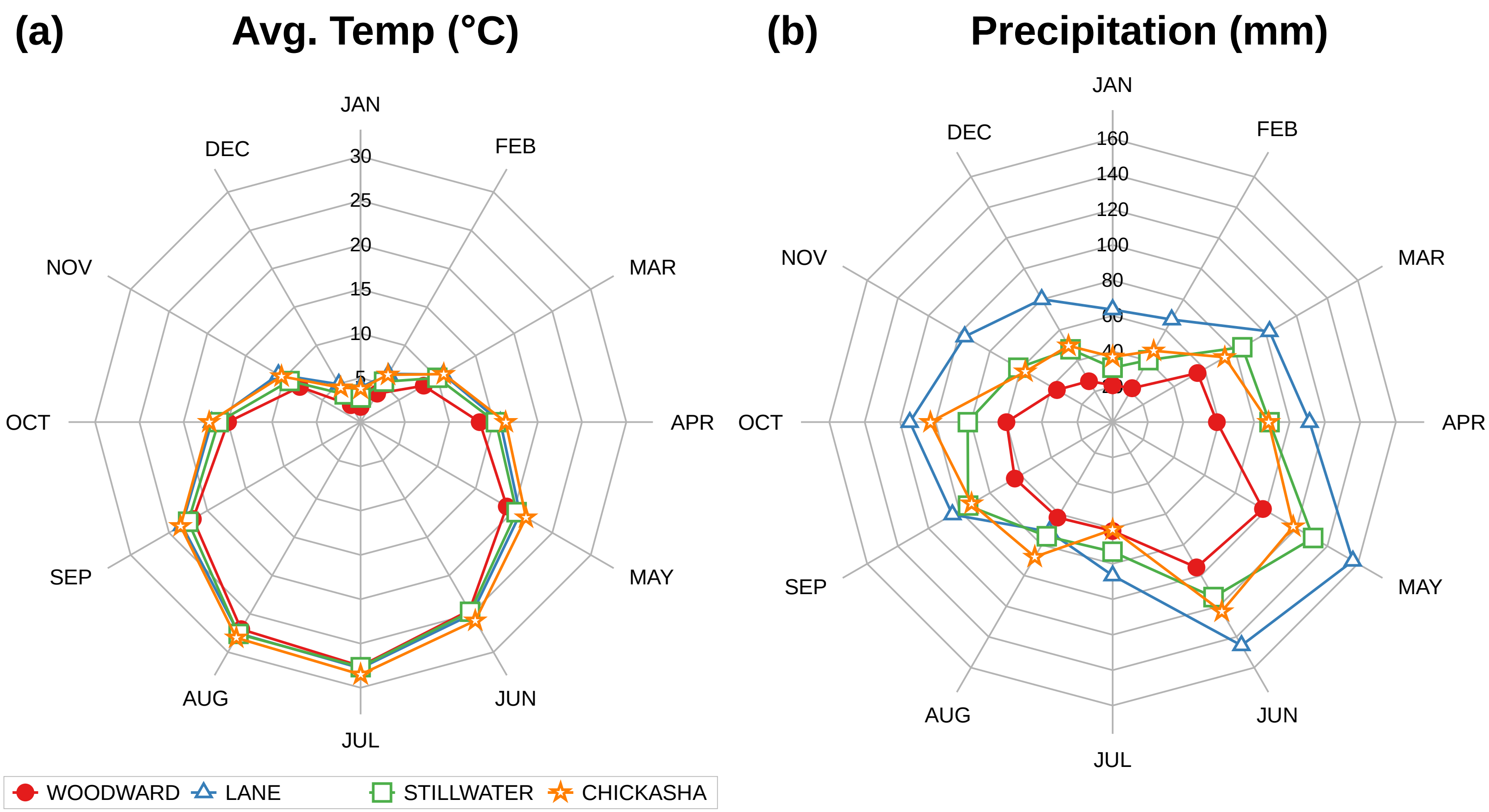

Fig. 1. Mean monthly temperature (°C) (a) and average total precipitation (mm) for four study locations (Lane, Stillwater, Chickasha, and Woodward) based on 30-year climate normal.

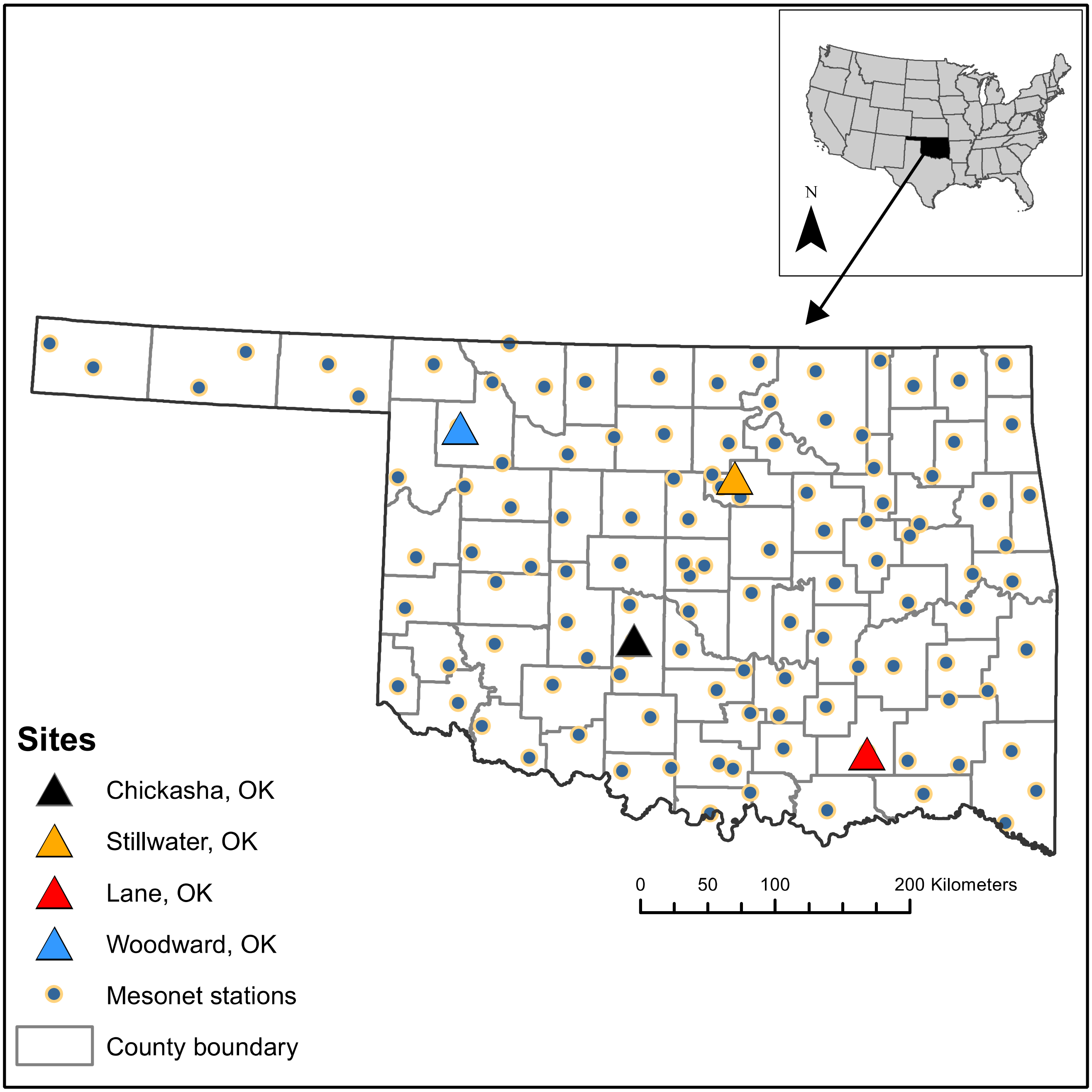

Fig. 2. Mesonet site distribution across Oklahoma. The black triangle is the site in Chickasha, Oklahoma, where empirical models were derived using Eddy flux measurements. Blue, yellow, and red triangles are the field-based biomass data acquired at Woodward, Stillwater, and Lane, respectively. Polar plots of (a) average temperature and (b) precipitation for Woodward, Lane, Stillwater, and Chickasha, respectively.

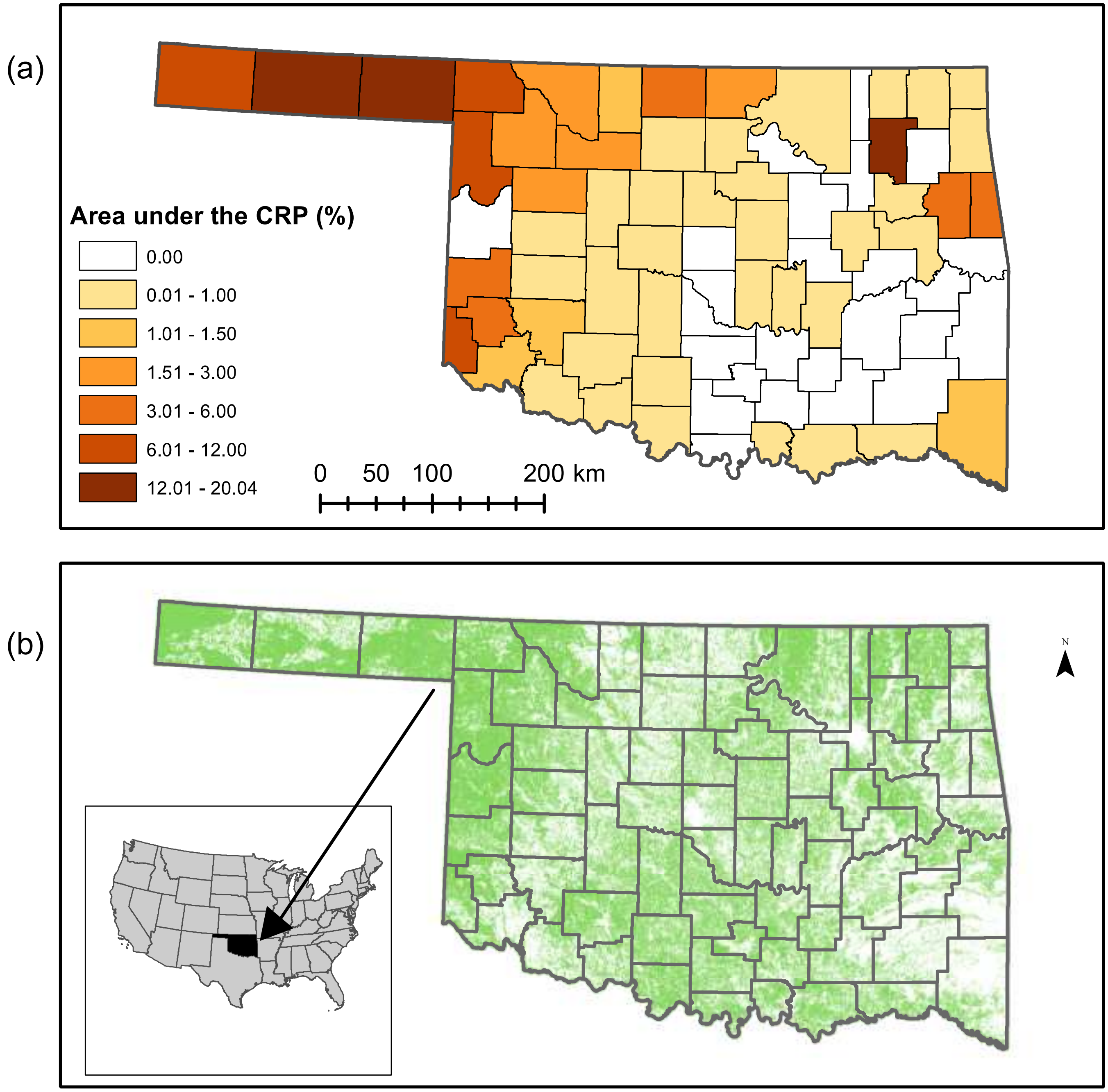

Fig. 3. Spatial distribution of the percentage of county area dedicated to the Conservation Reserve Program (CRP) in Oklahoma (a). Potential switchgrass production areas estimated by reclassifying the USDA-NASS Crop Data Layer 2008–2014 (b).

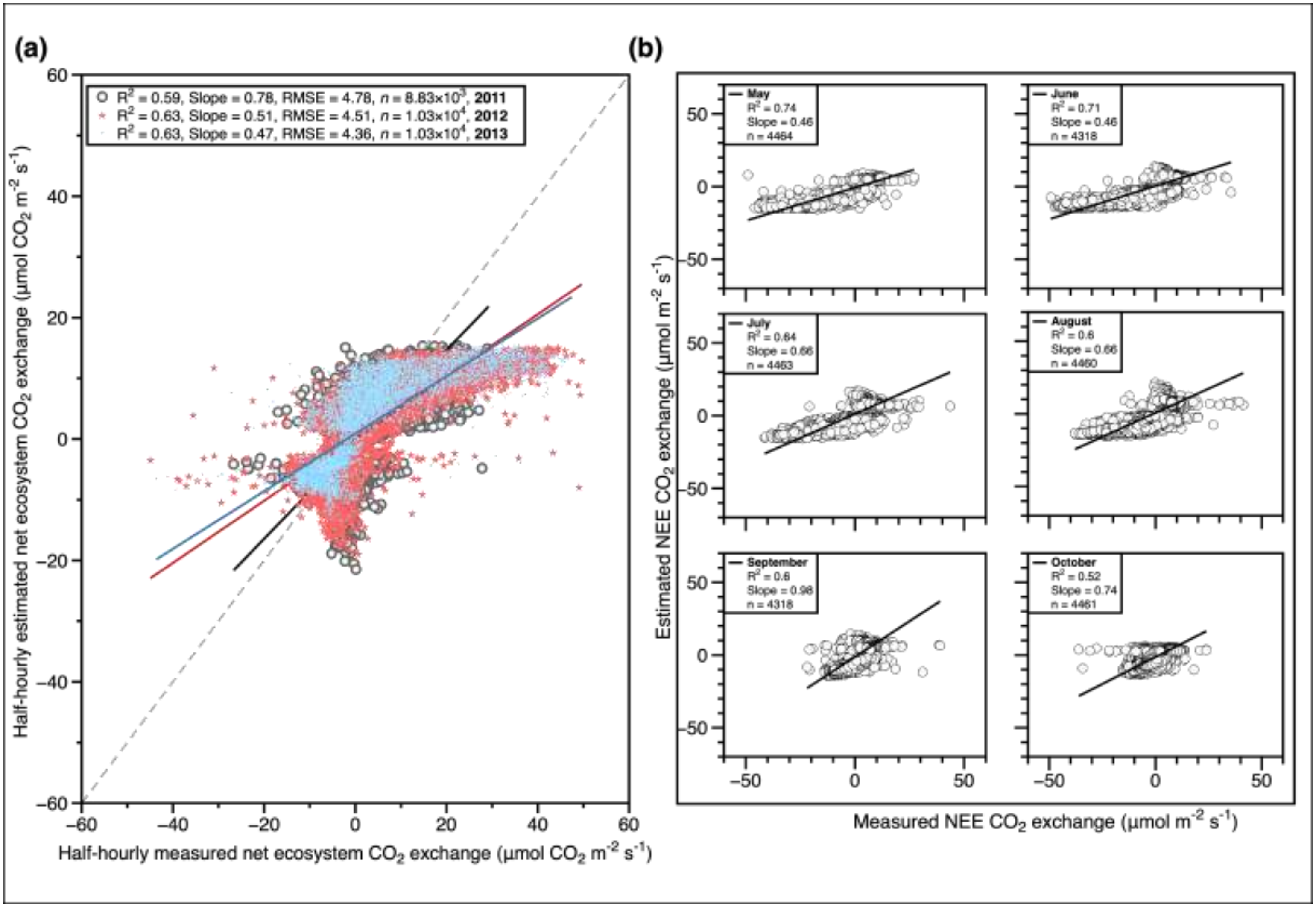

Fig. 4. (a) Comparison of empirical estimates of half-hourly net ecosystem CO_2 exchange (NEE) with measured half-hourly NEE for 2011, 2012, and 2013. The dotted black line represents a 1:1 relationship. (b) Comparison of half-hourly NEE with empirical NEE estimates for each of the individual months (May through October) of the active growing season.

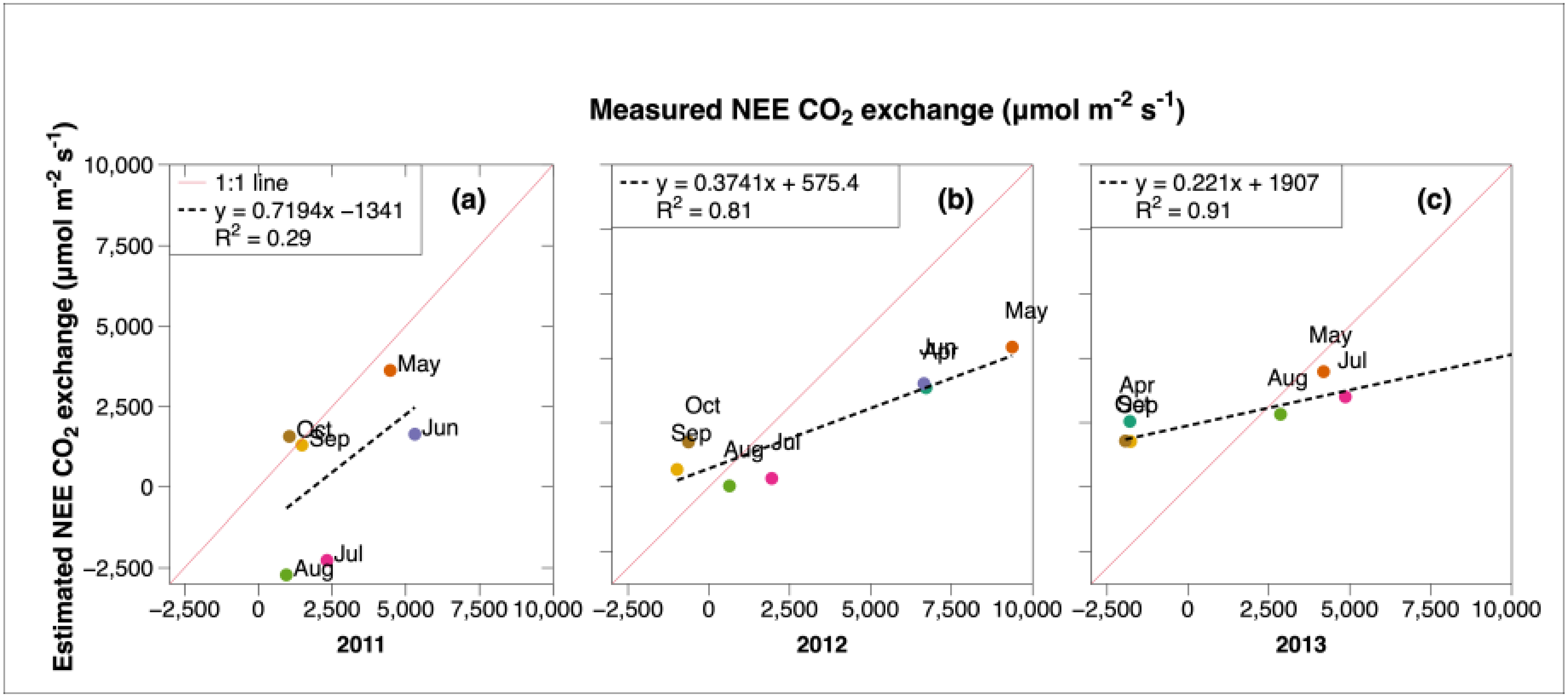

Fig. 5. Relationship between cumulative monthly measured and estimated net ecosystem CO_2 exchange (NEE) for Chickasha, Oklahoma in 2011, 2012, and 2013.

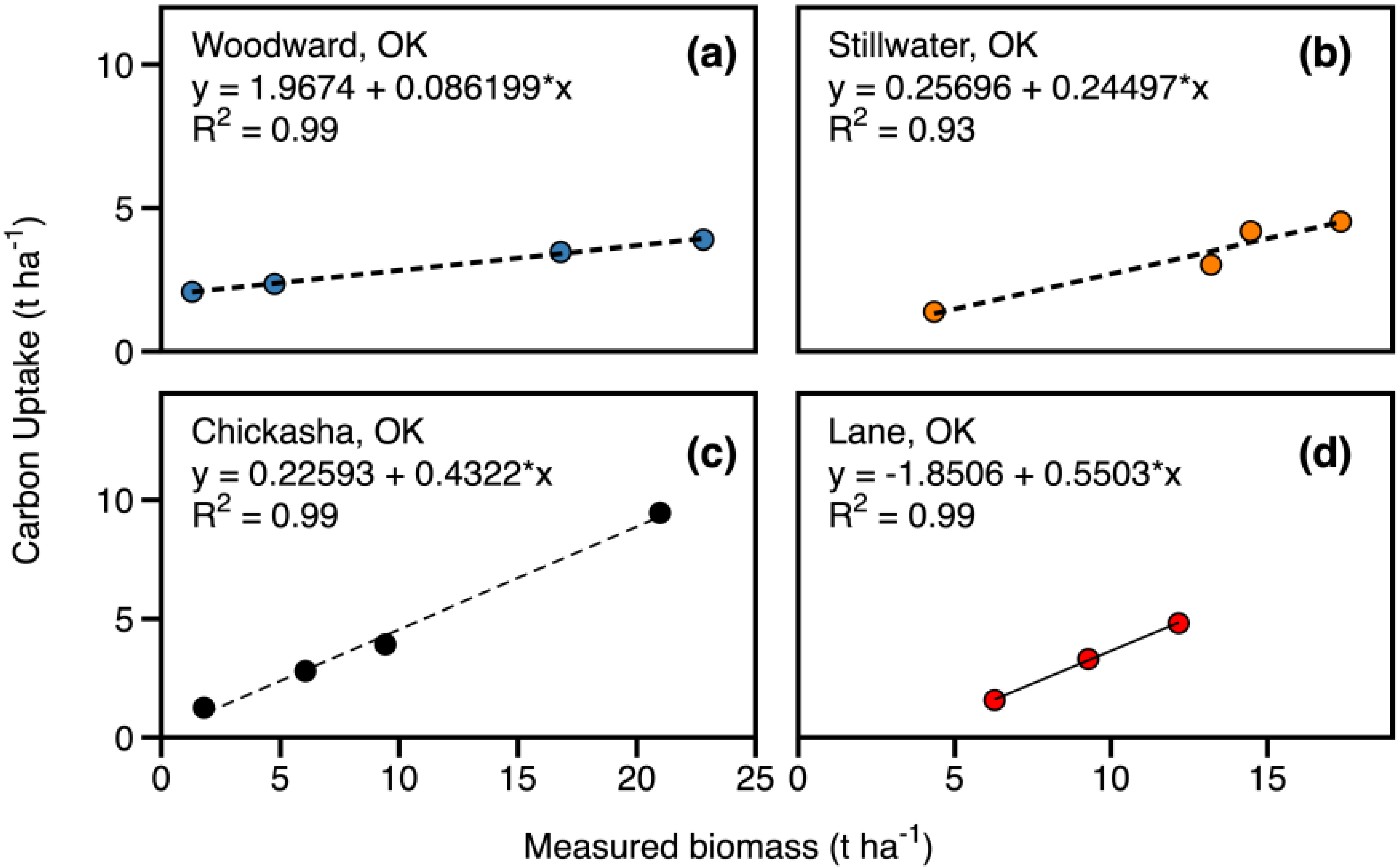

Fig. 6. Relationship between seasonal (April–October) carbon uptake (net ecosystem CO_2 exchange, t ha^{-1}) by switchgrass ecosystem and end-of-season aboveground switchgrass biomass for (a) Woodward, Oklahoma, (b), Stillwater, Oklahoma (c) Chickasha, Oklahoma, and (d) Lane, Oklahoma for 2011–2014. Biomass yield for Lane, Oklahoma for 2014 was not available.

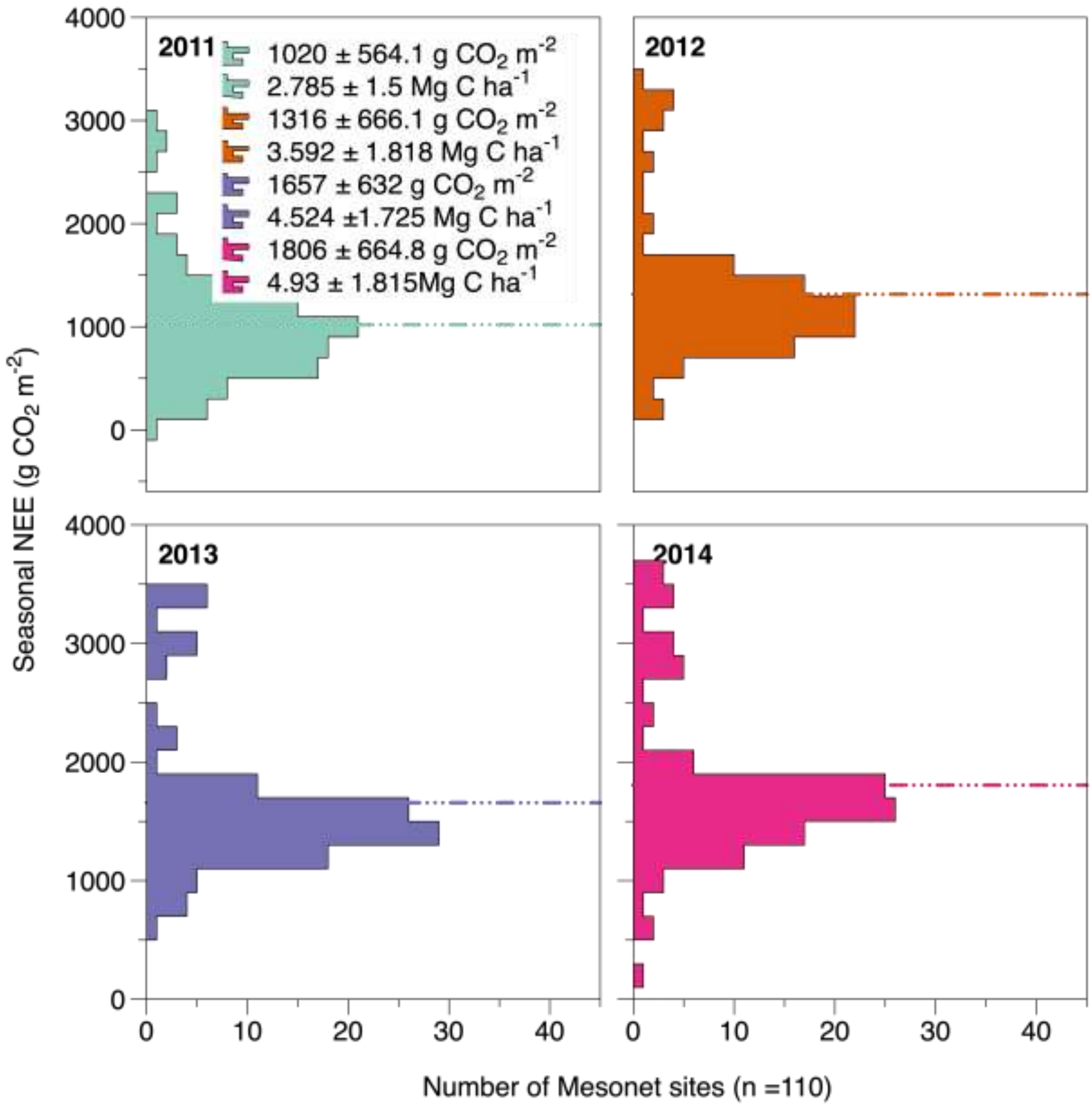

Fig. 7. Histogram of the seasonal net ecosystem CO_2 exchange (NEE) for the Mesonet sites for 2011-2014. Dashed lines represent the mean for the given year, and the legend shows the mean ± standard deviation of the seasonal NEE values across the Oklahoma Mesonet sites.

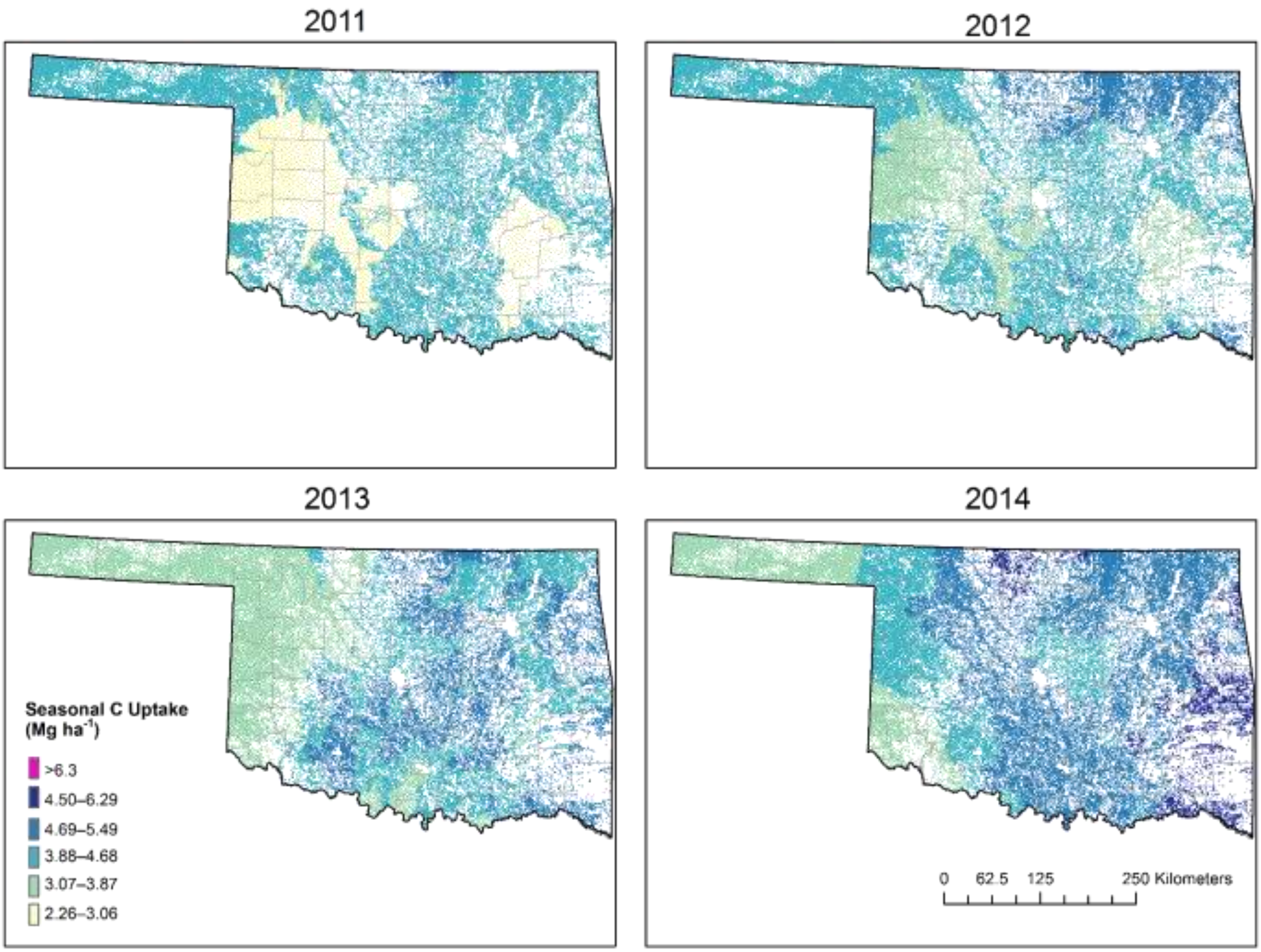

Fig. 8. Spatial explicit prediction of growing season net ecosystem CO_2 exchange (NEE) in a switchgrass ecosystem from 2011 to 2014 in a theoretical switchgrass production area across Oklahoma.