2015

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ARTICLE INFO

ABSTRACT

Accurate quantification and clear understanding of regional scale cropland carbon (C) cycling is critical for designing effective policies and management practices that can contribute toward stabilizing atmospheric CO_2 concentrations. However, extrapolating site-scale observations to regional scales represents a major challenge confronting the agricultural modeling community. This study introduces a novel geospatial agricultural modeling system (GAMS) exploring the integration of the mechanistic Environmental Policy Integrated Climate model, spatially-resolved data, surveyed management data, and supercomputing functions for cropland C budgets estimates. This modeling system creates spatially-explicit modeling units at a spatial resolution consistent with remotely-sensed crop identification and assigns cropping systems to each of them by geo-referencing surveyed crop management information at the county or state level. A parallel computing algorithm was also developed to facilitate the computationally intensive model runs and output post-processing and visualization. We evaluated GAMS against National Agricultural Statistics Service (NASS) reported crop yields and inventory estimated county-scale cropland C budgets averaged over 2000—2008. We observed good overall agreement, with spatial correlation of 0.89, 0.90, 0.41, and 0.87, for crop yields, Net Primary Production (NPP), Soil Organic C (SOC) change, and Net Ecosystem Exchange (NEE), respectively. However, we also detected notable differences in the magnitude of NPP and NEE, as well as in the spatial pattern of SOC change. By performing crop-specific annual comparisons, we discuss possible explanations for the discrepancies between GAMS and the inventory method, such as data requirements, representation of agroecosystem processes, completeness and accuracy of crop management data, and accuracy of crop area representation. Based on these analyses, we further discuss strategies to improve GAMS by updating input data and by designing more efficient parallel computing capability to quantitatively assess errors associated with the simulation of C budget components. The modularized design of the GAMS makes it flexible to be updated and adapted for different agricultural models so long as they require similar input data, and to be linked with socio-economic models to understand the effectiveness and implications of diverse C management practices and policies.

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1. Introduction

Agroecosystems not only provide essential life-supporting goods (e.g. food, fuel, livestock, and fiber) for humans, but also hold the promise to sequester carbon dioxide (CO_2) and other greenhouse gases (GHGs), thereby mitigating potential negative impacts of future climate change (Lal and Bruce, 1999; Paustian

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et al., 2006; Smith et al., 2007). The potential impact of changing farming practices for global emissions of GHGs has been widely recognized (UNEP, 2013). Agricultural technologies and practices can potentially mitigate ~5.5–6.0 Pg CO_2-eq yr^{-1} emissions at the global scale (Smith et al., 2007). The significant magnitude of this mitigation potential makes it necessary to consider physical, chemical, and biological dynamics of managed landscapes when understanding, quantifying, and regulating the global carbon (C) cycle (Moureaux et al., 2008; Sus et al., 2010).

The development of effective measures to stabilize atmospheric CO_2 concentration requires accurate quantification of the spatial variation and magnitude of C flux. Due to the lack of systematic and extensive collection of C budget observations, modeling approaches have been often used by researchers and decision makers (Saby et al., 2008; Ogle et al., 2010; West et al., 2010). A suite of modeling tools and methods operating at national or regional scales have been developed to estimate soil organic C (SOC) change and/or land-atmosphere C exchange by using inventory statistics, computer simulation models, satellite remote sensing products, geographic information systems, and/or eddy covariance flux tower measurements (Post et al., 2001; Whittaker et al., 2013). For example, an inventory method (West et al., 2008, 2010) was developed to estimate county-scale harvested biomass C, net primary production (NPP), SOC inputs and decomposition, and net ecosystem exchange (NEE), as well as agronomic production emissions of GHGs from seeding, tillage, fertilizer application, and harvesting. This inventory method is heavily rooted in the integration of U.S. Department of Agriculture's (USDA) National Agricultural Statistics Service (NASS) surveyed crop yields, State Soil Geographic (STATSGO) data (USDA-NRCS, 1995), and empirical relationships between SOC dynamics and diverse crop management practices derived from hundreds of field experimental sites. This data-rich and fine-scale approach has been recognized as a benchmark for cropland C budgets in several compelling model intercomparison and C budget synthesis projects, including the North American Carbon Program's (NACP) Midcontinent Mid-Continent Intensive (MCI) Campaign (Ogle and Davis, 2006; Schuh et al., 2013) and Regional Interim Synthesis (Hayes et al., 2012; Huntzinger et al., 2012). Despite the strength of the inventory approach in reliably quantifying the flux of C from ecosystems, the lack of detailed representation of the mechanisms regulating crop growth and development, water and biogeochemical cycling, and human interventions, limits its role in understanding the feedbacks among land use, climate change, and C cycling (Smith et al., 2012).

The study of complex agroecosytem relationships is best approached through process-based model analyses in combination with experimental data and field monitoring. Mechanistic agroecosystem models are being suggested as an important component of an integrated global framework for soil C monitoring and assessment (Smith et al., 2012). For example, a framework by Ogle et al. (2010) used the process-based CENTURY ecosystem model (Parton et al., 1994), operating at the monthly time step, to estimate SOC changes on the US croplands from 1990 to 2000. Their modeling system employed 121,000 National Resources Inventory (NRI) sampling sites across the US and integrated tillage practices, fertilization, soil types and edaphic characteristics, and climate variations. The point scale simulations were generalized to the scale of major land resource areas (MLRA) for reporting SOC change. The Environmental Policy Integrated Climate (EPIC) model (Williams, 1995) was tested at eighteen sites in Iowa and incorporated into a geospatial modeling system to simulate SOC change over the Iowa croplands (Causarano et al., 2008). Their modeling system used the Soil Survey Geographic (SSURGO) data that contains more detailed soil survey maps than STATSGO and a Landsat

based cropland map at a resolution of 30 m, but aggregated them into a composite layer of 250 m to explicitly define EPIC modeling units. They simulated a typical corn–soybean rotation characterized with three types of tillage practices at the state-level. Their simulations were evaluated against state-level NASS surveyed corn and soybean yields. These studies consistently demonstrated the importance of using mechanistic models and highlighted the promise of using fine-scale spatial and intensive management information for accounting cropland C budgets (Smith et al., 2012).

The continuous development of spatial data for climate, terrain, crop classification, and soils has resulted in dramatic increase in spatially-explicit information, thereby providing new opportunities to further advance the application of process-based models. However, as most management data, such as tillage and fertilization, are not available in a spatially-explicit way, it is risky to assume that the performance of these models at the site level transfers to the regional scales. Recent studies (Zhang et al., 2013b, 2014) showed that C flux simulated by process-based models is sensitive to the accuracy and completeness of crop management data, as well as the resolution of soil data. In addition, process-based models demand many more parameterization and data preparation efforts than inventory approaches, rendering them prone to more sources of uncertainty. The lack of extensive evaluation of the process-based models at the regional scales makes it difficult to assess their credibility for large-scale C budget estimates, thus limiting their role in developing effective C management practices.

Our objective, therefore, was to describe and test a geospatial agricultural modeling system (GAMS) that integrates the process-based EPIC model with spatially-explicit climate, soils, land use, terrain data, and surveyed crop management data (including fertilization, tillage, planting, and harvesting) to characterize cropping systems in the US Midwest. GAMS operates at a spatial resolution of 56 m that is consistent with the recently developed Crop Data Layer (CDL) (Johnson and Mueller, 2010). GAMS contains a Geographic Information System (GIS), a proven tool for geospatial data processing and management in regional scale environmental modeling (Rao et al., 2000; Schaldach and Alcamo, 2006; Liu, 2009; Wang et al., 2010). To facilitate model implementation and results processing at such a high resolution, it is also equipped with a parallel computing component and a relational database that is compatible with multi-threading model execution, data processing, and analysis.

We selected the US Midwest as the study area to examine the performance of GAMS (Fig. 1). Agroecosystems in the Midwest provide >85%, >80%, and >50% of total maize, soybean and wheat production in the entire US (USDA-NASS, 2011) and, concomitantly provide ~60%, ~45%, and ~20% of world trade in these crops (USDA-ERS, 2010). This highly productive agricultural area is a hotspot of cropland C sequestration in the US (West et al., 2010) and contains biofuel production activities aimed at enhancing energy security and GHG mitigation (EISA, 2007; NRC, 2011; USGCRP, 2012). These dimensions combined make the US Midwest an ideal test bed for applying and assessing GAMS.

As EPIC has been extensively tested for cropland C budget simulation at the site scale (e.g. (Wang et al., 2005; He et al., 2006; Izaurralde et al., 2006; Causarano et al., 2007; Izaurralde et al., 2007; Causarano et al., 2008; Apezteguía et al., 2009; Schwalm et al., 2010; Zhang et al., 2013b)), this research focused on assessing its performance at the county-scale against NASS-surveyed harvested biomass and cropland C budgets estimated by an inventory approach (West et al., 2010). Although this inventory method has been used as a benchmark in numerous model intercomparisons and C budget syntheses, its estimates of NPP, NEE, and SOC change have not been independently corroborated at the county scale with other process-based agro-ecosystem models.
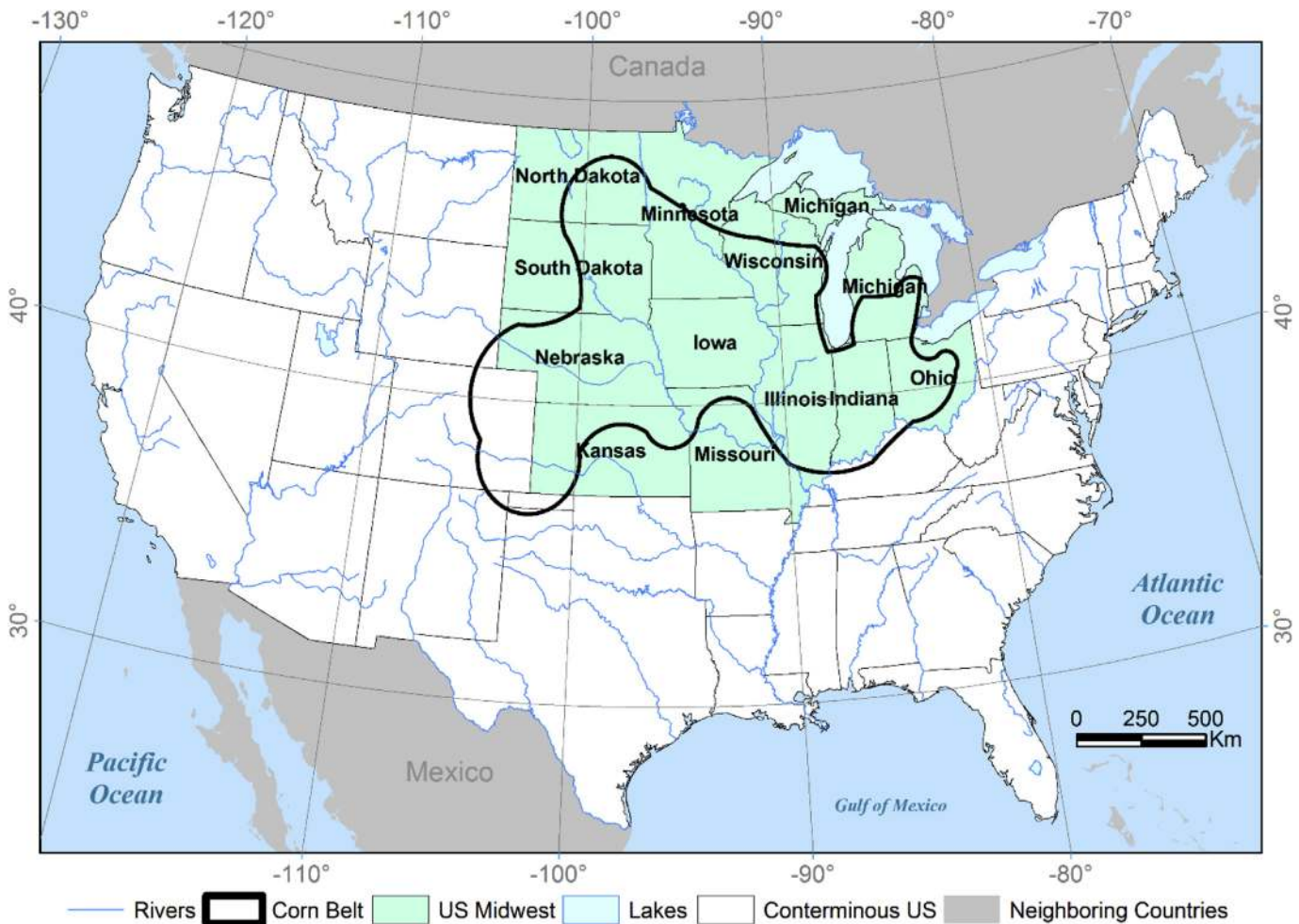
Fig. 1. Location of the study area. (The 12 states in the US Midwest show a high overlap with the Corn Belt. The extent of the Corn Belt is adapted from Liang et al. (2012)).

Thus, this comparison not only serves as an evaluation of the EPIC's county-scale estimates, but also provides an independent confirmation of the inventory method. Besides evaluating GAMS for multi-year average total cropland C flux, we also analyzed results for individual plant species and years. Overall, although GAMS exhibited a high degree of agreement with county-scale NASS crop yield data and inventory estimates (West et al., 2010), noticeable discrepancies were observed, particularly at the level of individual crop species and annual scale evaluations. Based on these spatial and temporal analyses, we identify possible causes for the inconsistencies and uncertainties in GAMS and discuss strategies for further enhancing its performance and promoting its uses in cropland C management.

2. Materials and methods

2.1. Overall framework design

GAMS contains three components (Fig. 2). A Geographic Information System (GIS) that fuses multi-source data to prepare spatially-explicit map units and derive each unit's climate, management, soil, land use, and terrain attributes. The employment of high-resolution land use and soil maps in defining homogeneous spatial modeling units (HSMUs) results in ca. 2 million units and ca. 15 million input–output files for cropland in the US Midwest. This requires supercomputing resources in order to efficiently execute EPIC and analyze results. These EPIC compliant input files are fed into a Python-based parallel computing package, which simultaneously employs hundreds of processors to execute EPIC on the Pacific Northwest National Laboratory's (PNNL) Evergreen computing cluster. The simulation variables are sorted out and stored in online PostgreSQL relational databases and can be easily queried and linked to geospatial data for thematic mapping,

summarization, and verification. The three components of GAMS are loosely coupled, rather than wrapped in an integrated software package. This flexible configuration allows GAMS to be modified and/or extended for other modeling exercises and analyses.

2.2. Description of EPIC

The EPIC model has been extensively tested for many agricultural cropping systems landscapes, and applied worldwide to examine agronomic and environmental impacts of alternative management practices and climate change (Wang et al., 2012). EPIC is a comprehensive terrestrial ecosystem model capable of simulating key biophysical and biogeochemical processes, such as plant growth and development, water balance, C and nutrient cycling, soil erosion, and greenhouse-gas emissions; and how these processes are influenced by climate conditions, landscape configurations, soil properties, and management practices. The plant growth sub-model of EPIC is a revised version of Crop Environment REsource Synthesis (CERES) (Williams et al., 1989; Jones et al., 1991), employing the concept of radiation-use efficiency by which a fraction of daily photosynthetically-active solar radiation is intercepted by the plant canopy and converted into plant biomass. Daily gains in plant biomass are affected by vapor pressure deficits, atmospheric CO_2 concentrations, nutrients availability, and other environmental controls and stresses. Currently, EPIC is parameterized for approximately 120 plant species including food crops, native grasses, and trees. EPIC's hydrology module contains all salient terrestrial water cycling processes including snowmelt, surface runoff, infiltration, soil water content, percolation, lateral flow, water table dynamics, and evapotranspiration. EPIC's biogeochemical module is a modified version of the CENTURY model describing decomposition and transformation of soil C and nitrogen (N) (Izaurralde et al., 2006) as regulated by many factors and processes, such as soil texture, pH, crop yields, atmospheric N input, fertilizer and manure, and tillage, among others.

The crop growth and SOC algorithms of EPIC have been examined against field observations from numerous sites across the world (Wang et al., 2005; He et al., 2006; Izaurralde et al., 2006; Causarano et al., 2007; Izaurralde et al., 2007;
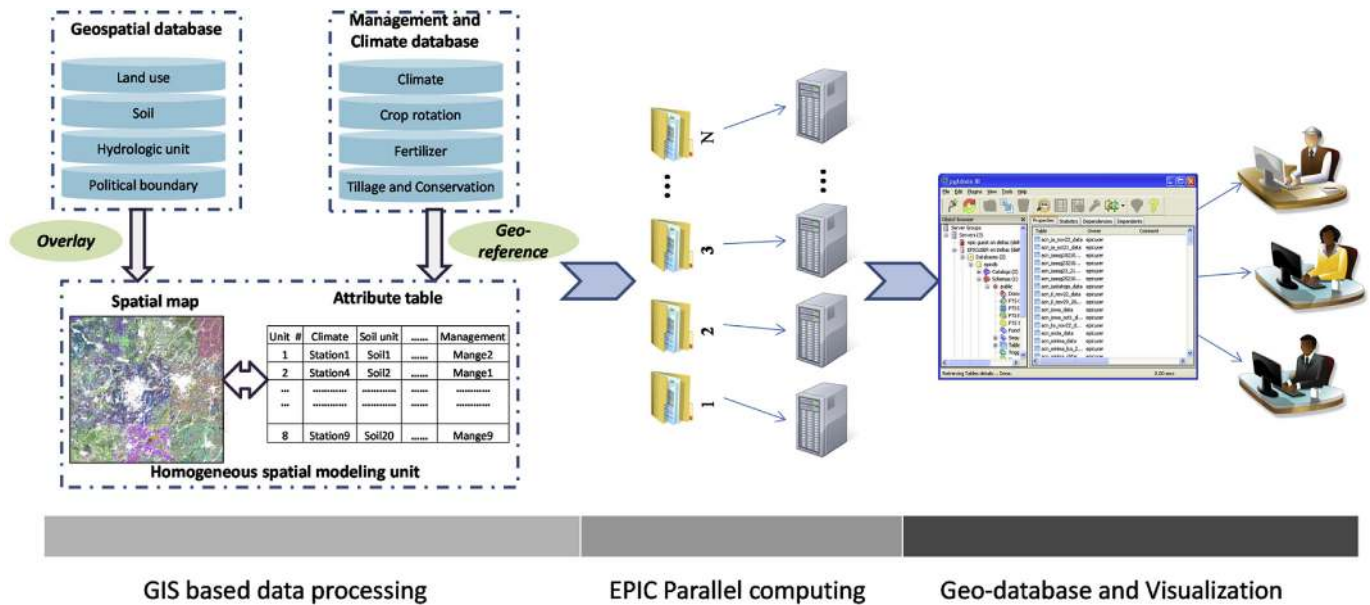
Fig. 2. Conceptual diagram of the geospatial modeling framework. (It contains a GIS system fusing multi-source data, a Python based parallel computing package, and relational database query and visualization functions.)

Causarano et al., 2008; Apezteguía et al., 2009; Schwalm et al., 2010; Zhang et al., 2013b). Its robust performance has made it a useful tool for assessing conservation effects of the Conservation Reserve Program (CRP) (USDA-FSA, 2008, 2010). Recent studies (Schwalm et al., 2010; Zhang et al., 2013) showed that the C algorithm in EPIC simulated well NEE of diverse agroecosystems in the Midwest, where NEE was calculated as heterotrophic soil respiration minus the net C sequestration from the atmosphere into plant biomass (i.e. NPP) and is opposite in sign to Net Ecosystem Production (NEP) (Chapin et al., 2006). A negative sign of NEE indicates C sequestration into biosphere, while a positive one denotes emission into the atmosphere. Here, we focus on the biogenic-related cropland C processes included in the NEE calculation but do not consider fossil fuel C emission from agronomic practices and heterotrophic respiration by humans and livestock (West et al., 2011).

Key parameters and initial state variables need to be determined before running models. One parameterization strategy that has been adopted in multiple model assessment and intercomparison projects (Schwalm et al., 2010; Srinivasan et al., 2010) consists of parameterizing variables based on prior information (e.g. from literature or field experiments) without attempting to extensively calibrate parameters to match observed variables of interest. In this case, model performance is highly dependent on the quality of input data. Therefore, we did not modify the default crop, hydrologic, and biogeochmical parameters within EPIC (Williams, 1995), but focused on deriving data-based agroecosytem parameters to characterize cropping systems across the Midwest US and using extensively state-of-the-art geospatial data to drive EPIC. Detailed description of the data used and parameterization procedures is presented in the following section.

2.3. Fusing spatially-explicit and multi-scale surveyed data into EPIC

We expanded the spatially explicit modeling system from the nine county area previously examined (Zhang et al., 2010) to operate across the entire US Midwest. In so doing, we performed the following efforts: processing SSURGO soil map and attribute data, replacing a uniform crop rotation pattern with spatially-explicit crop sequences derived from multi-year CDL data, and compiling North-American Land Data Assimilation System 2 (NLDAS2, ldas.gsfc.nasa.gov/nldas) climate data.

We compiled a series of geospatial databases, including land use/land cover, soil, catchment and political boundaries, and topography data, to define homogeneous spatial modeling units (HSMUs) and provide relevant parameters to drive the EPIC model. We used the following geospatial layers:

2.3.1. Crop rotation map

To create crop rotation maps for the US Midwest, we used a method developed using ArcPy in the ArcGIS environment to combine multi-year CDLs and select representative crop rotations (Sahajpal et al., 2014). We used four years of CDL data from 2007 to 2010 and for each state identified dominant rotation classes that account for over 85% of the spatial and temporal crop patterns in the US Midwest. This simplification lowered the total number of crop rotations from 115,425 to around 200, greatly reducing redundancy and computational burden at a relatively low cost inaccuracy.

2.3.2. Soils

The county-scale vector SSURGO maps downloaded from the US Department of Agriculture (USDA) Geospatial Data Gateway (datagateway.nrcs.usda.gov) were merged and converted into a raster format with a resolution of 56 m, consistent with the CDL. Soil properties processed for EPIC included the number of soil layers; layer depth; slope gradient and length; albedo; bulk density; pH; percent sand, silt, clay and coarse fragments; and percent organic C and total N.

2.3.3. Topography

The Shuttle Radar Topography Mission (SRTM), which produced a digital elevation model (DEM) for the region at a resolution of 30 m (Farr et al., 2007), provided elevation for EPIC to calculate atmospheric pressure.

2.3.4. Catchment and political boundaries

10-digit hydrologic units, and county and state boundaries were also used to define HSMUs, which were further linked to surveyed data to prepare EPIC inputs.

By overlaying the above geospatial layers, we obtained a spatial map composed of units with unique properties defined by the following dimensions: unique ID, latitude, elevation, slope, crop rotation, soil type, county, state, and hydrologic unit.

The geo-location information contained in each HSMU was used to geo-reference climate records and management practices at various scales. First, we used the latitude and longitude of each unit to locate the closest climatological grid of the NLDAS 2, which contains climate forcing data (temperature, precipitation, solar radiation, wind speed, and relative humidity) covering the US at an 8-km resolution. Second, we estimated annual N and phosphorus fertilizer application rates over 1991 to 2008 based on the state-level statistics from USDA (USDA-ERS, 2013). All counties within a state share the same fertilization levels. The fertilizer application rates differentiate between various crop species, but do not address variations for a crop species in different rotations. We derived planting and harvesting dates and heat units required by different crops to reach maturity from typical planting and harvesting dates of major crops in the U.S. provided by USDA (USDA-NASS, 1997) and using the potential heat unit program available at swat.tamu.edu/software/potential-heat-unit-program. We also filled gaps in annual fertilizer databases with the value from the closest year. Finally, at the county level, we derived the fractions of tillage practices compiled by the Conservation Technology Information Center (CTIC, 2008), which were re-processed into three categories: conventional tillage, conservation tillage, and no-till, and gap-filled for 2000–2008 (West et al., 2010). In order to cover the entire simulation period (1991–2008), we assumed that the spatial pattern of tillage practices for the initialization period (1991–1999) was similar to that averaged over 2000–2004. We allocated different tillage practices to each HSMU by assuming that farmers apply no-till and conservation tillage to steep soils in order to preserve soil productivity and protect the environment. Conventional tillage was assigned to flattest HSMUs, while no-till was applied to HSMUs with steepest slopes. The remaining HSMUs implemented conservation tillage.

Each HSMU of the composite layer possessed multi-dimensional information as illustrated in Fig. 2. The spatially-explicit scheme employed here allows us to preserve the spatial details of land use and soils patterns, while making it flexible for geo-referencing climate data and crop management practices and aggregating simulation results to the county-scale for comparison.

2.4. Parallelized EPIC execution and output data analysis

For the entire US Midwest, executing the over 2 million EPIC runs serially would need 5555.6 h or 231.5 days. This time consuming task necessitated the development of a parallel computing facility to improve the modeling efficiency. The parallel computing component of the GAMS was constructed by revising and re-structuring modules of software developed by Nichols et al. (2011); Zhang et al. (2013a). It seamlessly combines Python (python.org), mpi4py (Dalcin et al., 2011) and OpenMPI (www.open-mpi.org) to make use of hundreds of processors simultaneously. The architecture of the parallel computing package was similar to that depicted in Zhang et al., 2013a, except that it executed EPIC instead of the Soil and Water Assessment Tool (SWAT) (Arnold et al., 1998). It first identifies a Master processor among those allocated to a submitted job and splits the entire EPIC runs into a specified number of folders. Next, the Master processor sends commands to the remaining processors to execute EPIC in each of the folders in parallel. The parallel computing package extracts, organizes, and uploads EPIC simulated agronomic and environmental variables stored in millions of text files into an online PostgreSQL relational database to facilitate data query, analysis, and visualization.

2.5. Model performance assessment

In alignment with the previous inventory based cropland C budget estimates by West et al. (2008), (2010), we executed EPIC from 1991 to 2008, with 1991–1999 as an initialization period, and focused on comparing spatial patterns of modeling variables averaged over 2000–2008 at the county scale. We compared our modeling results with two types of data to assess its credibility and identify gaps for further improvements. The first type of data was the county-scale crop yield survey data from USDA-NASS' Quick Stats (quickstats.nass.usda.gov) from 1991 to 2008. The second type of data was derived from an inventory model, which calculates C in harvested biomass by multiplying NASS county crop yield with a C content factor of 0.45; estimates NPP as a function of C in harvested biomass, harvest index and root-shoot ratio; and calculates SOC changes by considering organic matter input, tillage, initial SOC concentration, SOC saturation, and the number of years in cultivation.

Two metrics that have been widely used in model assessment (Moriasi et al., 2007) were employed here: percent bias (PBIAS) (Gupta et al., 1999) and Pearson product-moment correlation coefficient (R) (Pearson, 1895). PBIAS is calculated as:

$$PBIAS = \left(\frac{\sum_{k=1}^{T}(f_k - y_k)}{\sum_{k=1}^{T} y_k} \right) \times 100 \tag{1}$$

where f_k is the model simulated value at a time unit or location k, y_k is the corresponding benchmark data value, and T represents the total pairs of data. PBIAS measures the average tendency of the simulated data to be larger or smaller than their observed counterparts. Note that, due to cancellation, a result of zero does not necessarily indicate low error (Bennett et al., 2013). Therefore, instead of examining a single aggregated PBIAS, we also derived PBIAS for each location (here at the county scale) and visually presented these values to detect geographic distribution of model performance.

The formula for calculating R is:

$$R = \frac{\sum_{k=1}^{T}(y_k - \bar{y})(f_k - \bar{f})}{\left[\sum_{k=1}^{T}(y_k - \bar{y})^2 \right]^{0.5} \left[\sum_{k=1}^{T} \left(f_k - \bar{f} \right)^2 \right]^{0.5}} \tag{2}$$

where $\bar{y}$ is the mean of benchmark data for the entire time period or across all sites under evaluation, $\bar{f}$ is the mean of simulated data. R measures the correlation of the measured and modelled values and indicates how well the model explains the variance in the observations. R ranges between +1 and −1, with 1 indicating total positive correlation, 0 denoting no correlation, and −1 representing total negative correlation. We calculated R to analyze the performance of GMAS to reproduce spatial patterns of cropland C budgets averaged over multiple years and at the annual scale. The joint use of PBIAS and R helps depict a fuller picture of the model performance in terms of both relative error and preserving the data pattern (Bennett et al., 2013).

3. Results and discussion

3.1. Evaluating EPIC simulated cropland carbon budgets against USDA-NASS surveyed crop yield and inventory based C estimates

With the inventory estimates of total C in harvested biomass, we observed concentrated areas of harvested biomass and associated regional C sinks in the study area (Figs. 1 and 3a–b). GAMS captured this spatial pattern with an R value of 0.89 (Fig. 4a). As crop yield represents a significant portion of total biomass production and the crop yield-to-total biomass ratio does not vary much geographically, the spatial distribution of NPP is similar to that of harvested C (Fig. 3c–d). Not surprisingly, the inventory estimates and EPIC simulations of NPP agree favorably with each other with a high correlation of 0.90 (Fig. 4b), though these two methods derive total biomass production with fundamentally different approaches. Summed over the cropland in the Midwest US, EPIC slightly underestimated total crop yield compared to NASS data (164 TgC yr^{-1} vs 172 TgC yr^{-1}), but overestimated total NPP by about 20% (499 TgC yr^{-1} vs. 401 TgC yr^{-1}) as compared to the inventory based estimate. This is likely related to the difference in how harvest index is determined in these two approaches. Although the maximum harvest index in EPIC is the same as those used by West et al. (2008), the actual harvest index used at harvesting is lower, because EPIC considers impacts of environmental stresses, including water and nutrients, and reduces the harvest index accordingly. The smaller harvest index in EPIC resulted in higher estimated NPP, even though EPIC underestimated crop yield.

The close match regarding crop yield and NPP indicates that these two methods estimated similar amounts of residue inputs into soils, which were calculated as NPP minus harvested C. However, this did not translate into a close correspondence between the simulated SOC change patterns by these two methods (Fig. 3e–f; Fig. 4c); though they agreed on the total SOC change (~14 TgC yr^{-1} sequestration predicted by EPIC vs. ~12 TgC yr^{-1} by the inventory method). A closer look at the spatial distribution of SOC change reveals a wider variability in the EPIC results versus the inventory based estimates. EPIC simulated county-scale SOC change ranges from ~−80,614 to ~270,012 MgC county^{-1} yr^{-1}, which compares to a much narrower range between ~ −43–~107,292 MgC county^{-1} yr^{-1} of the inventory method. This contrast is related potentially to the more variable spatial details represented in the EPIC modeling system, which includes finer soils, land use, and climate forcing. For example, EPIC used SSURGO (with a scale 1:24,000) for soil properties, CDL to map crop rotation, and NLDAS climate inputs with a resolution of ca. 8 km, while the inventory method derived SOC change from STATSGO (with a scale 1:250,000) and does not account for climate forcing variability.

Regarding NEE, the relatively smaller magnitude of SOC change as compared with harvested C rendered the pattern of NEE dominated by the distribution of harvested C (Fig. 3g–h). Not surprisingly, we achieved a high correlation (R of 0.87) between the two sets of NEE estimates (Fig. 4d). EPIC estimated an annual cropland C flux of ~−272 TgC yr^{-1}, which is much greater in magnitude than the NEE of ~−185 TgC yr^{-1} estimated by the inventory method. This difference is primarily caused by the discrepancy between NPP estimates, which influences residue inputs into soils and respired C flux into the atmosphere.

At the annual scale, harvested C, NPP, SOC change, and NEE estimated by EPIC also showed positive correlation with those estimated from the inventory method, but the spatial agreement deteriorated compared to the assessment using data averaged over 2000–2008 (Fig. 5). For example, the average annual correlation from 2000 to 2008 is ca. 0.73 for harvested C, lower than the R value of 0.89 calculated using the multi-year average crop yield data. Generally, EPIC's performance improved over time, with average performance over 2000–2008 better than that over 1991–1999. The relatively poor performance during 1991–1999 may be related to the unstable equilibrium in SOC due to incomplete initialization and the lack of accurate crop management data. Notably, the GAMS simulations can be extended beyond 2000–2008 for long-term estimates when climate and crop management data are provided.
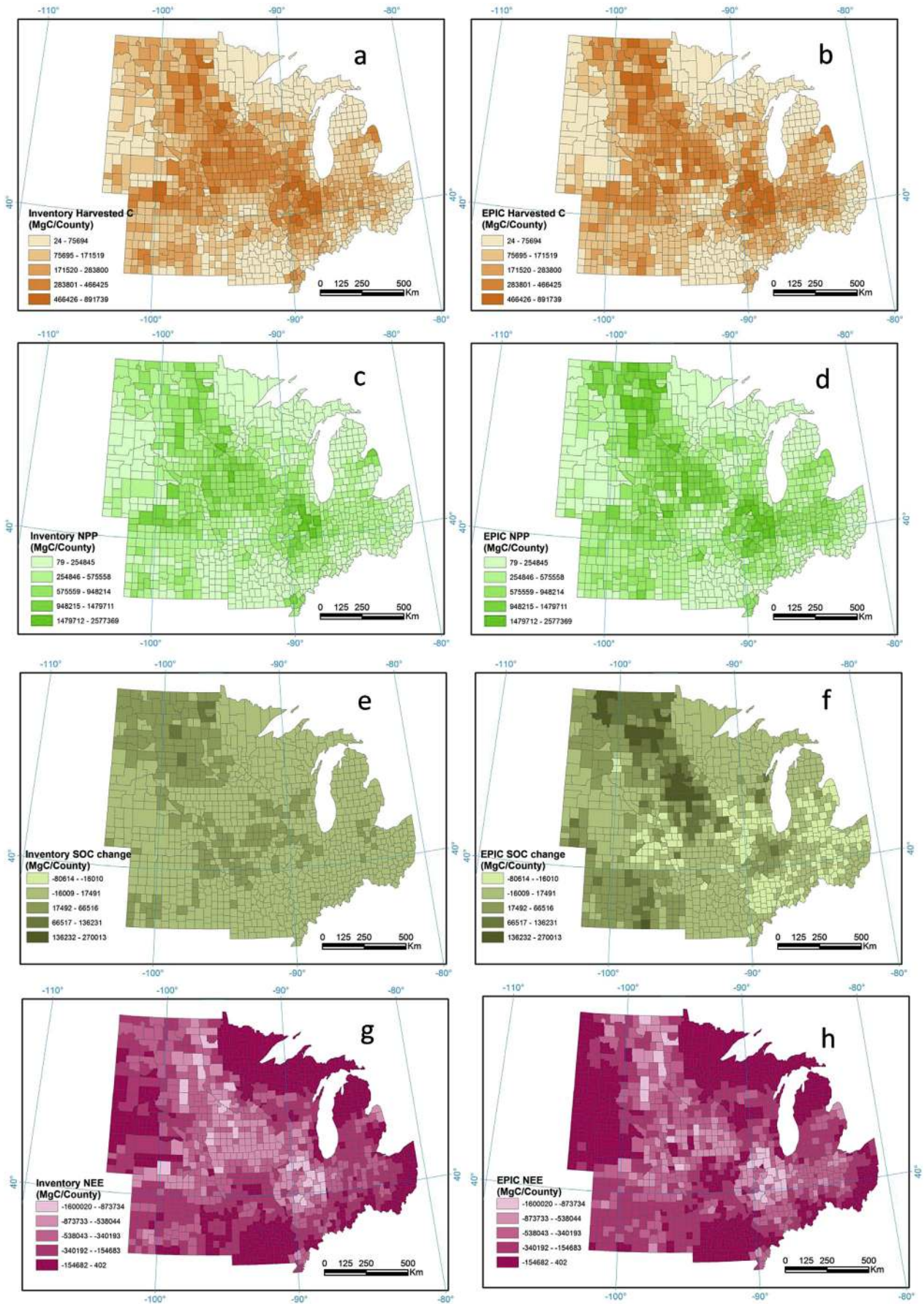
Fig. 3. Multi-year average (2000–2008) spatial comparison between EPIC simulated and inventory estimated cropland carbon budget components. (Left panel presents results from the inventory method by West et al. (2010); Right panel includes EPIC simulated variables).
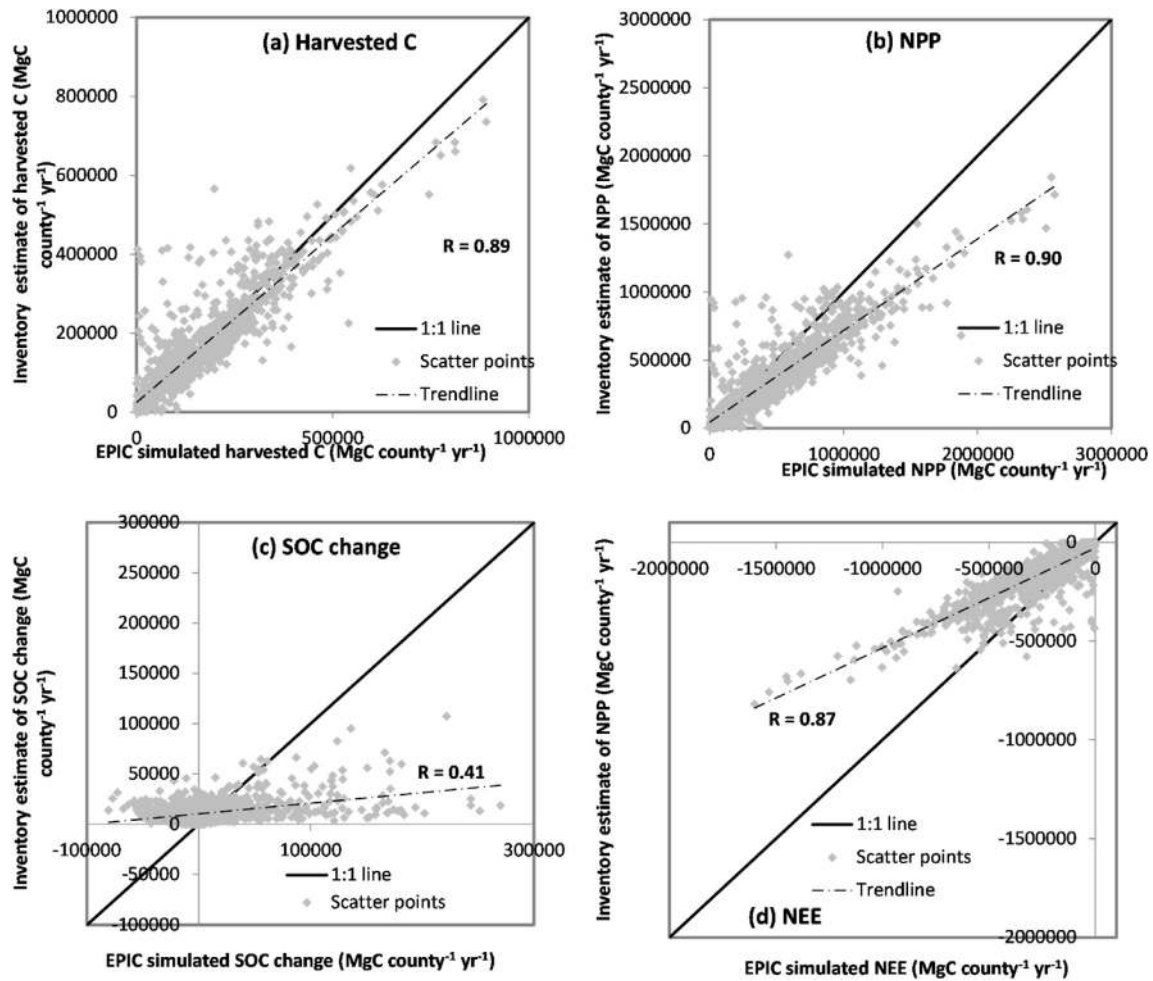
Fig. 4. Spatial correlation between EPIC simulated and inventory estimated multi-year average (2000–2008) cropland carbon budget components.

Overall, the corroboration between the inventory method and GAMS highlights the robustness of GAMS for simulating county-scale cropland C budgets as influenced by a suite of interacting climatic, edaphic, hydrologic, and anthropogenic factors. Meanwhile, as an independent estimate of cropland C budgets, the EPIC results also confirmed the reliability of a widely used inventory method (West et al., 2008, 2010). However, the comparisons also raised the disagreement between EPIC and the inventory method for SOC change and NEE, deserving further analysis.

3.2. Individual species comparison between EPIC simulated and NASS surveyed crop yields

The results presented in Section 3.1 compared cropland C budgets aggregated across all crop species in the US Midwest (West et al., 2010). This aggregated assessment provides little information on the performance of EPIC for each crop species. We further examined the performance of EPIC for reproducing spatial patterns of each of the six major crop species, including corn, soybean, winter wheat, spring wheat, alfalfa, and sorghum (Figs. 6 and 7). Two types of assessments were conducted: [1] spatial correlation between EPIC simulated and NASS reported crop yield averaged over 2000–2008, and [2] annual spatial correlation over 1991–2008.

Corn and soybean, the two most planted crops in the US Midwest, have higher yield in the central and eastern states than in the northern states of the US Midwest. EPIC preserved this NASS reported pattern (Fig. 6a–d). Notably, EPIC tended to substantially under-estimate corn and soybean yield in western Nebraska and Kansas, while exhibiting large positive biases in eastern Kansas, much of Missouri, and part of Indiana. For counties in other states, the yield bias in general fell between −30% and +30% (Fig. 9a–b). When excluding the two heavily irrigated states (i.e. Nebraska and Kansas), we observed a noticeable increase in spatial correlation between EPIC simulated and NASS reported corn and soybean yield. For corn, correlation increased from 0.42 when all states data were used (R_all) to 0.72 when excluding Kansas and Nebraska (R_rainfed) (Fig. 8a). Similarly, R_rainfed for soybean (0.78) was much higher than R_all (0.48) (Fig. 8b).

For winter wheat, we observed a poor performance of EPIC for capturing NASS reported spatial yield distribution (Fig. 6e–f), with R_all of 0.19 and R_rainfed of 0.42 (Fig. 8c). For about half of the counties with winter wheat production, EPIC simulated yield bias was either less than 40% or over 40%, with the greatest under- and overestimations in Kansas and North Dakota, respectively (Fig. 9c).

For alfalfa, EPIC overestimated alfalfa yield averaged over 2000–2008 in northern Wisconsin, southern Illinois, and the southeast of Kansas by 50%, while under-estimating yield in western Nebraska and Kansas by 40% (Fig. 7a–b; Fig. 9d). We also observed significant increase in spatial correlation between EPIC simulated and NASS reported alfalfa yield by excluding Nebraska and Kansas, with R_all of 0.34 and R_rainfed of 0.77 (Fig. 8d).
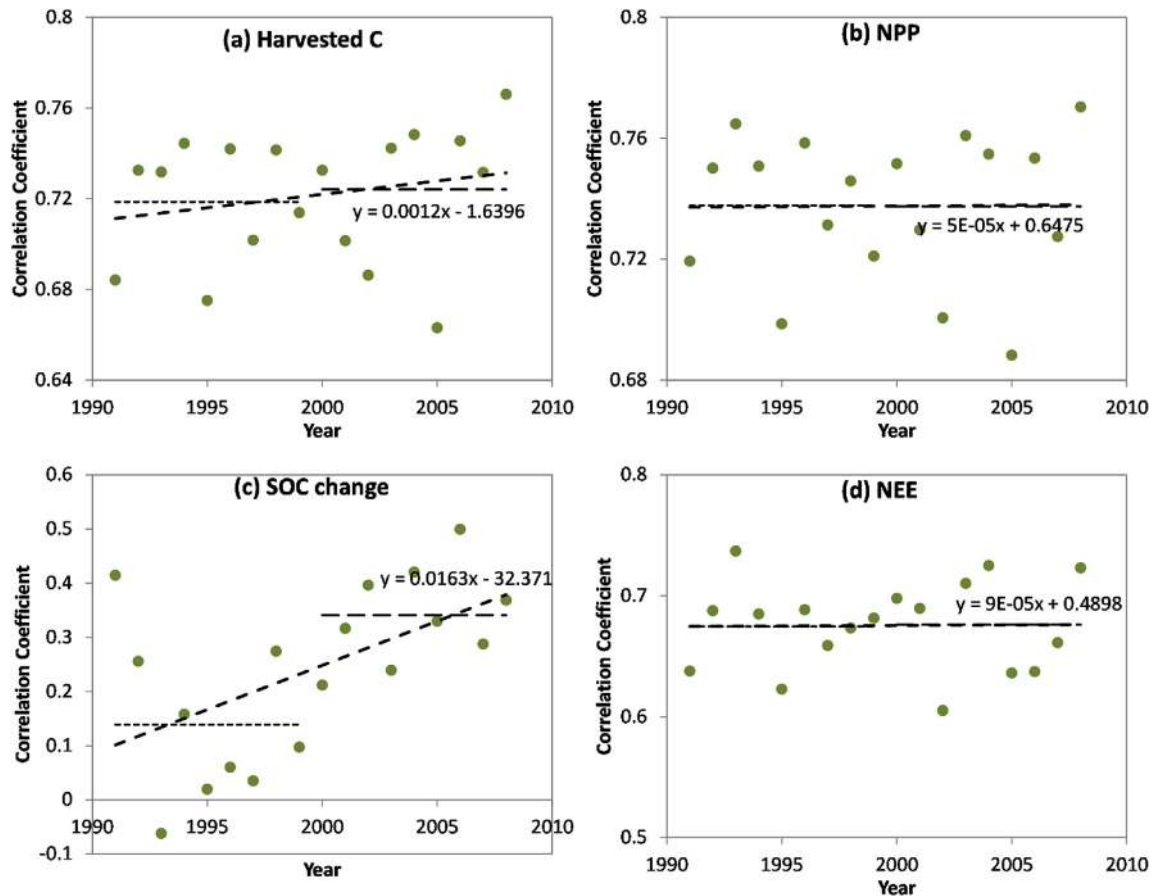
Fig. 5. Time series of annual spatial correlation between EPIC simulated and inventory estimated cropland carbon budget components over 1991–2008.

The spatial domains of spring wheat and sorghum are more localized compared with the other four crops; with sorghum mainly present in Kansas and spring wheat in North Dakota and much of Minnesota (Fig. 7c–f). For spring wheat, EPIC captured its spatial yield pattern well with an *R* value of 0.83 (Fig. 8e), the highest among all six crops. The bias of EPIC simulated, spring wheat yield was between −30% and +30% for most counties, but reached 50% in eastern North Dakota and several counties in middle Minnesota (Fig. 9e). For sorghum, we also observed a close match between the spatial distribution of the EPIC simulated and NASS reported yield as indicated with an *R* value of 0.73 (Fig. 8f), as well as an overestimation of crop yield in most counties (Fig. 9f).

For the multi-year average assessment, the crop yields simulated by EPIC explained the dominant spatial pattern at the county scale reported by NASS for all six crops (Figs. 7 and 8). However, we also observed pronounced overestimation and underestimation in the eastern and western parts of the evaluation domain, respectively (Fig. 9). The failure to adequately simulate irrigation management in Nebraska and Kansas significantly compromised the performance of EPIC in these two states. By excluding them, we observed a noticeable increase in spatial correlation (at least 0.23) between EPIC simulated and NASS reported crop yield for the four widespread crops (i.e. corn, soybean, winter wheat, and alfalfa) that spanned across both rainfed and irrigated regions. In most counties of the ten states dominated with rainfed cropping systems, we observed either moderate underestimation or overestimation (Fig. 9a–d), with overestimation as the major pattern for all six crops except sorghum. For some counties, overestimation reached over 50%. An extreme case is spring wheat, for which EPIC

overestimated crop yield by 50% for about half of the counties within the spring wheat domain. The optimistic prediction by EPIC for rainfed regions is possibly caused by the inadequate consideration of the negative effects of pest damage and excess water on crop growth, among other factors.

We also extended the multi-year average assessment of EPIC to an annual scale for the period of 1991–2008 (Fig. 10). In general, EPIC performed better in the later years than in the early years of the simulation period for all six crops, highlighting that completeness and accuracy of input data play a crucial role in reliable agroecosystem modeling. This is consistent with previous findings obtained at the site scale that EPIC performed better for sites with complete and detailed agronomic data than for those sites without detailed management information (Zhang et al., 2013b). EPIC's annual performance (Fig. 10) is in general comparable to the multi-year average assessment (Fig. 8). The average annual spatial correlation over 2000–2008 is close to the spatial correlation calculated with multi-year average crop yield. When excluding Nebraska and Kansas, we also obtained increased spatial correlation similar to that shown in Fig. 8.

3.3. Assessing accuracy of simulated cropland area used in GAMS simulations

Accuracy of the geospatial modeling system is heavily dependent on the CDL and SSURGO. When overlaying CDL and SSURGO to define HSMUs, the final cropland area used by EPIC is determined by both the accuracy of CDL and the completeness of soil properties in SSURGO. We found a high correlation between the county-scale
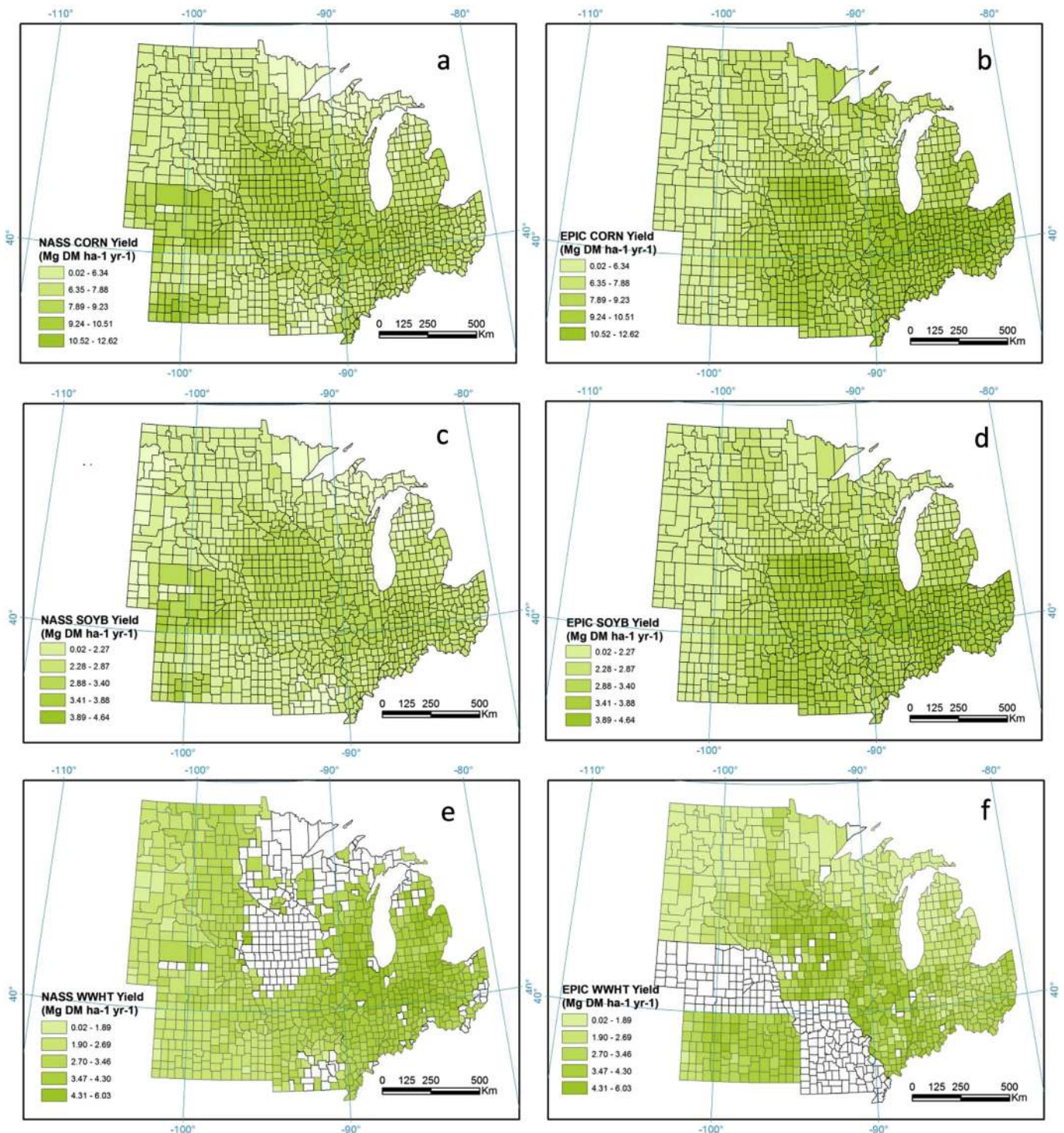
Fig. 6. Spatial distribution of species-specific crop yield averaged over 2000—2008 for corn (a—b), soybean (c—d), and winter wheat (e—f). (GAMS overestimates winter wheat's extent in Iowa and Minnesota, and northern Wisconsin. In contrast, the crop rotation map used in GAMS leaves out winter wheat in Nebraska and Missouri. This is because we simplified crop rotations derived from multi-year CDLs, which merges crop rotations with minor areas into dominant ones. The winter wheat area in these two states represents less than 8% of the total cropland area, leading to its omission.)

cropland area used by EPIC and those from NASS (Fig. 11). The US Midwest cropland area simulated by EPIC was about 72 million ha, approximately 6.5% lower than the NASS surveyed area of 77 million ha. Notably, in the US Midwest, the total alfalfa in NASS is ca. 4.3 million ha, which is much higher than the simulated alfalfa area of only 1.6 million ha. This was mainly caused by the low accuracy

of CDL for alfalfa identification (USDA-NASS, 2014), which underestimated alfalfa by 40—50%. In addition, we discarded numerous small HSMUs that only accounted for about 2% of the total cropland area, but comprised about 2 million units. These factors, in conjunction with missing complete soil parameter sets for EPIC runs on a small portion of the cropland area, resulted in an overall
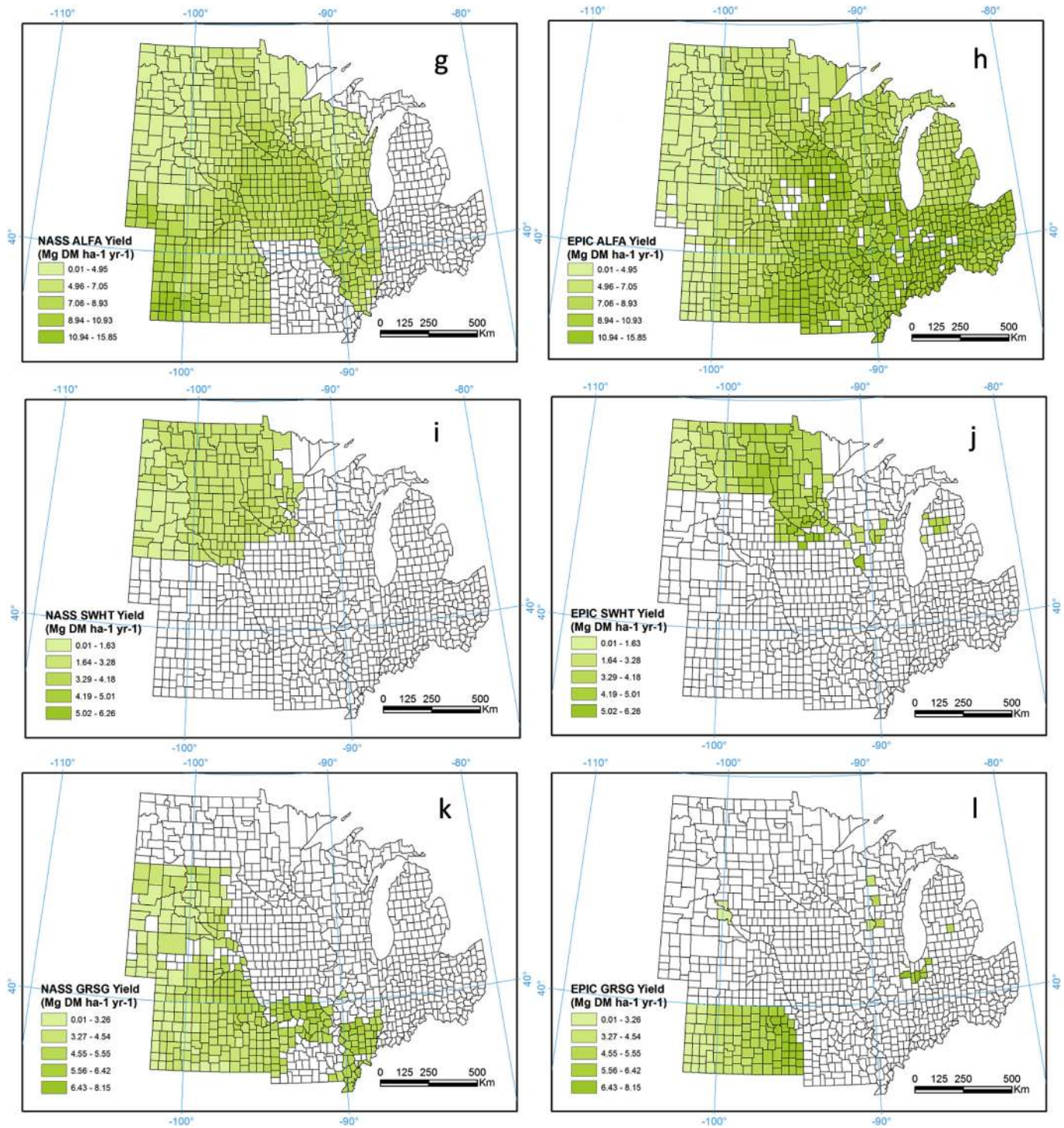
Fig. 7. Spatial distribution of species-specific crop yield averaged over 2000–2008 for alfalfa (g–h), spring wheat (i–j), and sorghum (k–l). (The NASS started to report alfalfa yield and area data in 2009 for Missouri, Indiana, and Ohio; therefore (g) does not show the presence of alfalfa in these states; The underestimation of spring wheat in South Dakota is because it is a minor crop and was removed during the process of simplifying crop rotation; similarly the missing extent of sorghum in South Dakota and Nebraska is also due to the crop rotation simplification that results in the loss of crops with small area).

underestimation of cropland area in the US Midwest by 5 million ha. The cropland area underestimation in part explains why we over predicted crop yield per unit area (Figs. 7–9) but still simulated well total crop yields. With future updates of the SSURGO database and refinement of CDL, we expect to see further improvement in geospatial representations of the agricultural landscapes in the US Midwest.

An individual plant species analysis indicated that simulated cropland area closely matched the corresponding NASS data for corn, soybean, and winter wheat, but alfalfa area was pronouncedly underestimated (Fig. 12). Compared to NASS data averaged over 2000–2008, the simulated cropland area across the US Midwest was overestimated by 13% and 17%, respectively, for corn and soybean, and underestimated by 8.4% for winter wheat. For alfalfa, our
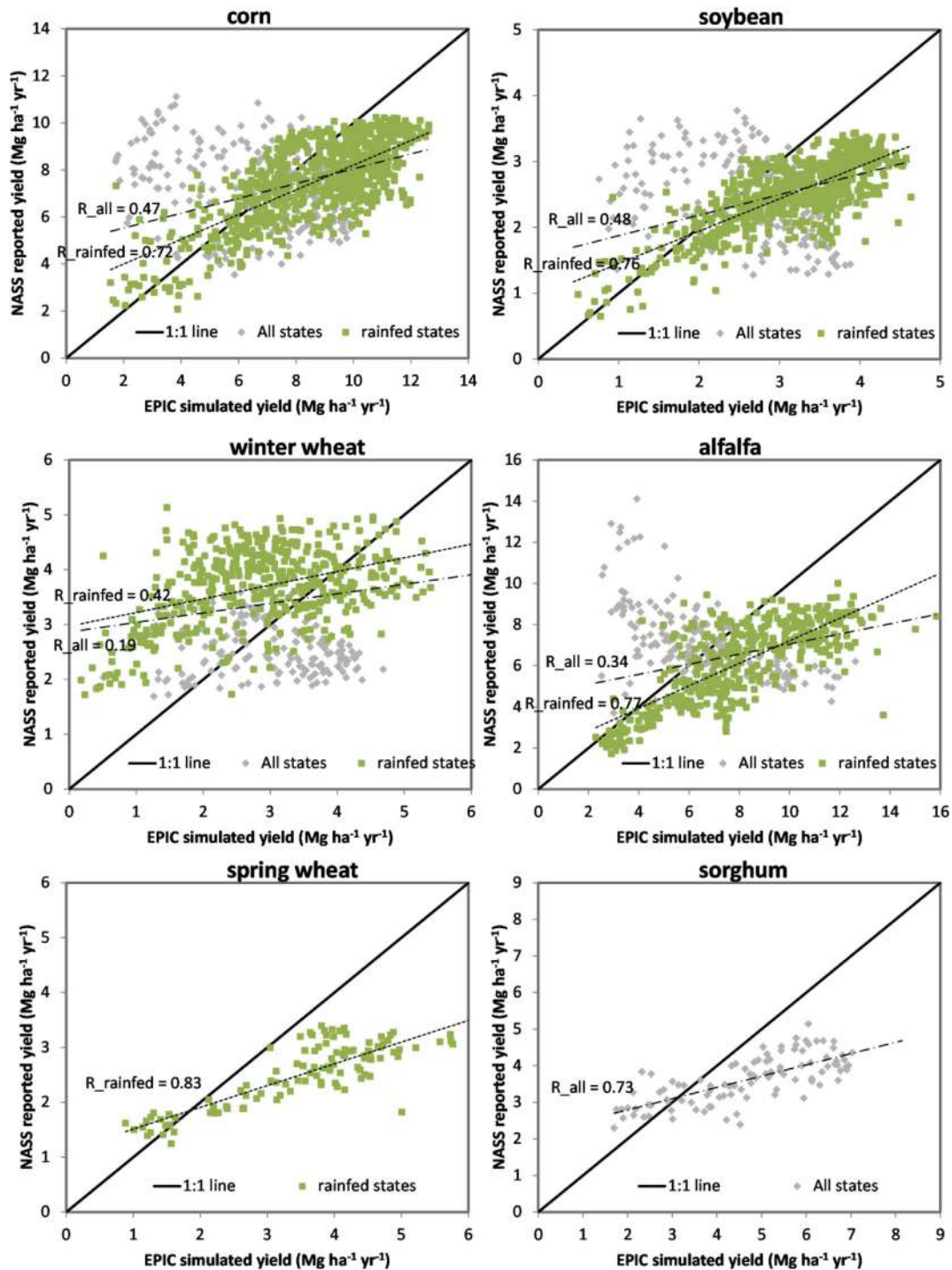
Fig. 8. Spatial correlation between EPIC simulated and NASS reported multi-year average (2000—2008) species-specific crop yield. (R_all is calculated with data from all counties, while R_rainfed is derived from counties other than Kansas and Nebraska).

simulated area was about 60% lower than that reported by NASS. In addition, our modeling system significantly overestimated spring wheat area while underestimating sorghum area. These accuracy metrics are in general poorer than those reported for CDL (USDA-NASS, 2014), which may be caused by the simplification of crop rotations with the aim of reducing the complexity of preparing EPIC required crop management files and the number of HSMUs (Sahajpal et al., 2014). As mentioned above, we identified over 2 million HSMUs for EPIC simulations. Without crop rotation

simplification the number of HSMUs would reach over 7 million, greatly increasing the computational cost and data storage burden. Cropland area under corn and soybean increased because they represent dominant crop rotations and certain crop rotation types with small shares were merged into them during the simplification procedure.

For the two locally concentrated crops (spring wheat and sorghum) significant biases in crop area were identified. Simulated spring wheat area was 34% higher than the NASS reported area,
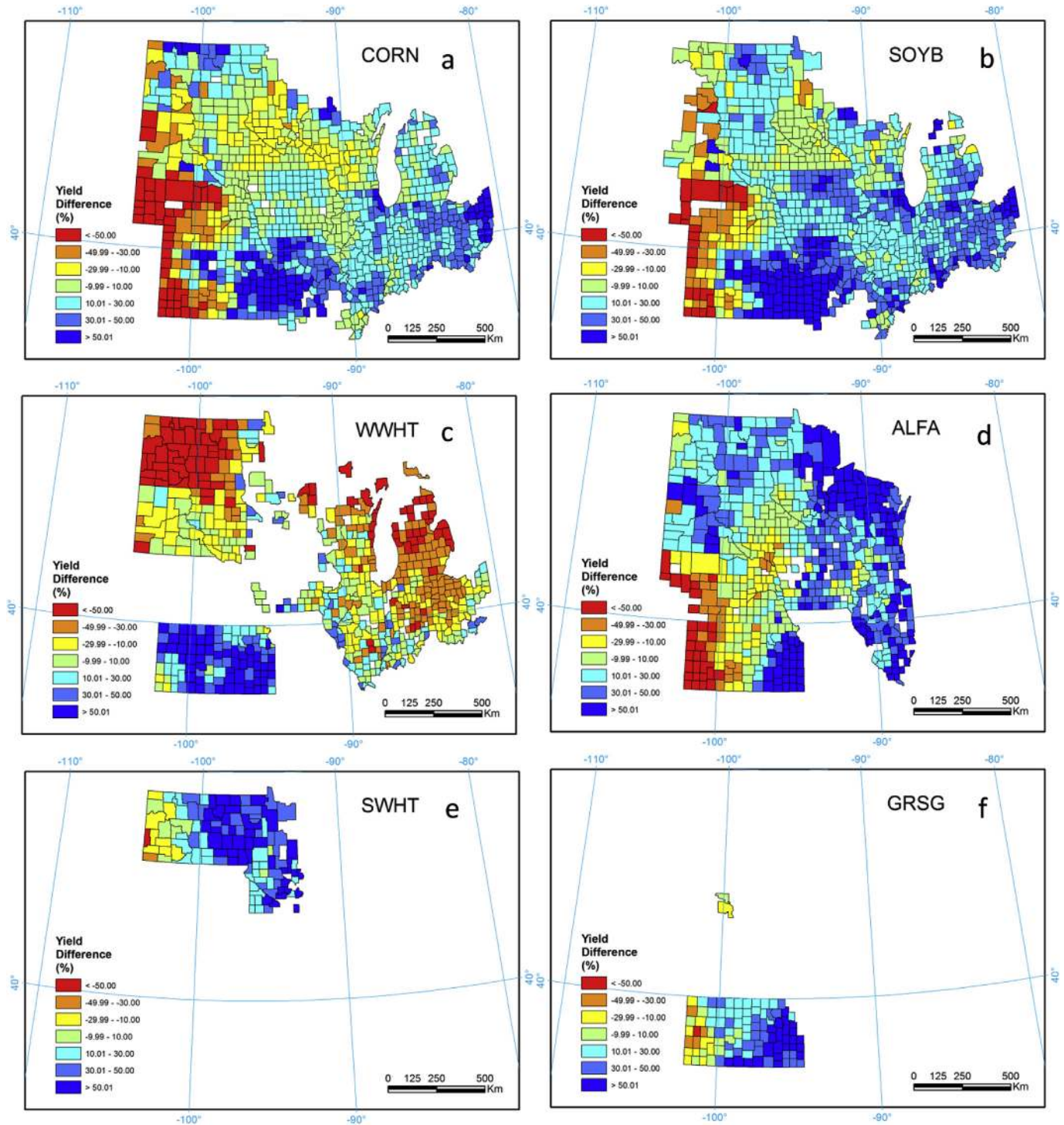
Fig. 9. Spatial distribution of species-specific bias in EPIC simulated multi-year average (2000–2008) crop yield. (Only those counties with concurrent EPIC simulated and NASS reported data are shown.)

while simulated sorghum area was about 60% lower. Our rotation simplification scheme expands dominant rotations while diminishing minor ones (Sahajpal et al., 2014). In North Dakota, spring wheat was a dominant crop species that accounts for ca. 34% of total cropland of 7.8 million ha, but a minor crop species covering only ca. 9% of the total cropland area (6.4 million ha) in South Dakota. As the simplified crop rotations in South Dakota preserved only ~80% of the accuracy of CDLs, we omitted all the spring wheat

in South Dakota (Fig. 7i–j). Crop rotations simplification caused shrinkage of sorghum area in Nebraska and South Dakota, because its acreage accounted for only 1.9% and 2.0% of the total cropland area in Nebraska and South Dakota (Fig. 7k–l), respectively, leading to merging of sorghum-involved rotations into other representative ones. Similarly, acreage of sorghum was ca. 1.2 million ha or 13.8% of the total cropland in Kansas, making it a minor rotation and thus a significant loss of sorghum area.
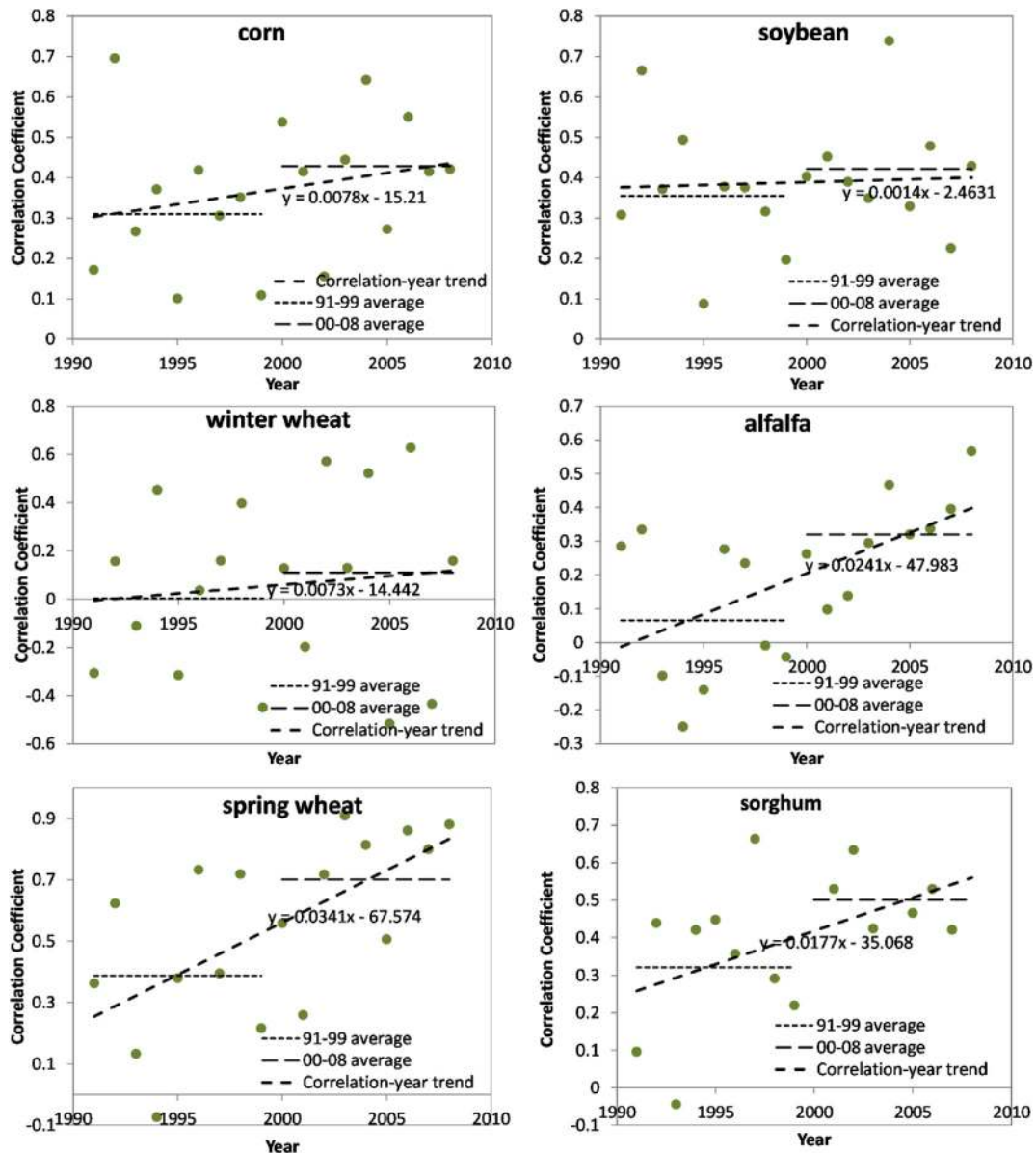
Fig. 10. Time series of annual spatial correlation between EPIC simulated and NASS reported species-specific crop yield over 1991–2008.

An annual-scale analysis also showed higher accuracy of simulated crop area for corn, soybean, and winter wheat than for alfalfa, spring wheat, and sorghum (Fig. 13). A clear accuracy improvement over time was observed for all crops, as we derived crop rotations using CDLs from 2007 to 2011 and assumed this crop rotation pattern was the same for years before this period. This trend, to some extent, explains the improved performance of EPIC for simulating crop yield over time (Fig. 10). Furthermore, these high annual correlation coefficients between simulated and NASS reported cropland area testify to the value of the GAMS for annual scale cropland C flux estimates.

3.4. Discussion

Overall, GAMS, as described and tested here, successfully simulated crop yields and cropland C budgets. The correlation between EPIC and the inventory method was close to 0.9 for harvested C, NPP, and NEE for multi-year average comparison, and was larger than 0.65 at the annual scale. We also identified notable discrepancies between the EPIC simulated crop yields and C fluxes and those either reported by NASS or estimated with a widely used inventory method. Below we elaborate on possible causes of these disagreements and discuss potential opportunities for further improving GAMS to support sustainable C management.

3.4.1. Possible explanations for the discrepancies between EPIC simulated and NASS reported crop yields

For the six crops simulated here, crop yield overestimation was the dominant pattern, except for winter wheat. For corn, soybean, alfalfa, spring wheat, and sorghum, EPIC generally underestimated crop yields in the west while overestimated crop yields in the middle and the east of this region. The underestimation in western Nebraska and Kansas was primarily due to the failure to adequately simulate the effects of irrigation, a key practice boosting crop production in these areas. The lack of spatial representation of species-specific irrigated farms, irrigation schedule, and irrigation
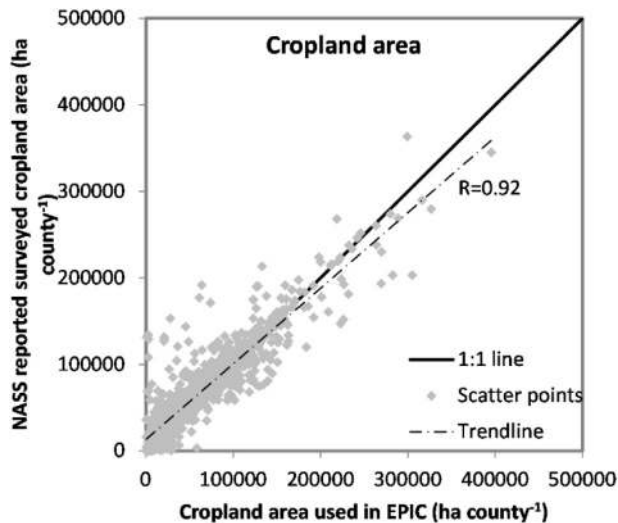
Fig. 11. Spatial correlation between simulated and NASS reported multi-year average (2000–2008) total cropland area.

volume impeded us from incorporating irrigation into GAMS in a consistent way. Irrigation changes plant growth and water availability, which in turn affects plant litter inputs and microbially-mediated SOC decomposition, thereby altering net cropland C flux. Therefore, integrating detection of irrigated areas by remote sensing and locally surveyed, irrigation management information promise to help improve simulations of crop yields and C budgets.

We did not identify any obvious reasons behind EPIC's over-estimation of crop yield. A literature review on previous applications of EPIC revealed that EPIC tended to over predict crop yield on rainfed land (Thomson et al., 2005b). Possible explanations are diverse, such as inadequate considerations of pest damage, detrimental effects of excess soil water, and competition between staple crops and weeds, as well as unrealistically optimistic simulation of biophysical parameters (such as leaf area index). Additionally, uncertainties arise from errors in soil data, climate forcing, and management schedule, including inaccurate planting and harvesting dates, extending state-level fertilizer application to each county, approximation of the timing of fertilization and tillage, and idealized allocation of county-scale tillage fractions. All these sources of uncertainties interact with each other and propagate through the processes simulated in EPIC, making it a challenge to identify the mechanisms responsible for EPIC's performance. To address this challenge, new data with refined quality and details (both spatial and temporal) and improved understanding of relevant agroecosystem processes and their robust mathematic representation in models are required. How to characterize and quantify these sources of uncertainties remain a challenge and require further research.

Similar to previous studies, we found that EPIC has difficulties for simulating winter wheat yields (Asseng et al., 2013). In general, winter wheat yield was underestimated in the northern area while overestimated in the southern part of the US Midwest. We derived three major crop rotations containing winter wheat, i.e. corn–soybean–winter wheat in the northern states and winter wheat-fallow and corn-winter wheat in the southern states. Winter wheat distinguishes itself from other annual crops because it is planted in fall and harvested in late spring or early summer of next year. We encountered some difficulties in preparing crop rotation management files that involve winter wheat. The typical planting date is usually earlier than the typical harvesting date of other annual crops such as corn and soybean, while its typical harvesting date is often later than the planting date of other annual crops. We had to shrink the length of growing seasons of both winter wheat and other annual crops in rotation by delaying planting and shift harvesting date earlier. This midway solution may deteriorate EPIC's performance for both winter wheat and other annual crops, with greater negative effects on winter wheat simulations because it is always impacted by such a compromise while other annual crops do not suffer when they are not in rotation with winter wheat. In addition, the varying performance of EPIC in Kansas as compared to that in the northern areas for winter wheat might be related to the crop species rotated with winter wheat. In Kansas, winter wheat often alternates with fallow, while in other areas it is usually in rotation with other crops. These factors interact with many other aforementioned uncertainties and require further systematic analysis.

3.4.2. Mismatch between EPIC simulated and inventory estimated SOC change

Of the estimated ~5.5–6.0 Pg CO_2-eq yr^{-1} GHG mitigation potential of agricultural technologies and practices at the global scale, approximately 89% comes from soil C sequestration (Smith et al., 2007). Therefore, diagnosing the discrepancies between EPIC simulated and inventory estimated SOC change is important for improving the understanding of the potential of soils in the US Midwest for GHGs mitigation.

We believe the major cause for the difference between EPIC simulated and inventory estimated SOC change lies in the fundamentally distinct approaches used to calculate SOC dynamics. EPIC explicitly considers microbially mediated, soil organic matter (SOM) dynamics as influenced by an array of biotic and abiotic factors, such as the quantity and quality of the plant litter inputs (e.g. lignin and cellulose content), soil texture, water content, temperature, oxygen availability, and the physical and chemical structure and composition of SOM, among others. In order to adequately simulate these processes, EPIC needs inputs of climate forcing, physical and chemical soil properties, and crop management practices (e.g., fertilizer, tillage, planting, and harvesting). In contrast, the inventory method estimates SOC change by considering its empirical relationship with initial SOC, residue input, tillage practice, length of cultivation, and SOC saturation. These two approaches suffer from different sets of uncertainty factors. EPIC uncertainties arise from errors in climate records, inaccurate soil parameters, incomplete management information, and interactions among these factors. Although the inventory method suffers less from input data and parameter errors, it relates SOC change with several control factors instead of systematically examining SOC dynamics as regulated by the joint impacts of all controls. This renders it susceptible to uncertainties arising from extrapolating site-scale observations to regional-scale estimates.

Another cause of the mismatch is the inaccurate representation of crop rotations in GAMS. As noted in Section 3.3, the CDL-derived alfalfa area is substantially underestimated in GAMS; the simplification of crop rotation brought enormous computation benefits but at the cost of the accuracy of different crop species. These mis-representations of crop species undermine simulated NPP, harvested biomass, and residue input into soils, as well as SOC change. In addition, we did not explicitly consider corn silage and sorghum silage, because CDL does not distinguish between the uses of these two crops for grain and silage. Due to a higher harvest index (more biomass is removed from field) for silage crops, plant residue inputs into soils and SOC sequestration are likely to be discounted. However, this simplified treatment of corn silage and sorghum silage seems to have minimal impacts on simulation results of SOC and NPP, as corn silage and sorghum silage account for only 4.7% and 2.4% total corn and sorghum acreage, respectively.
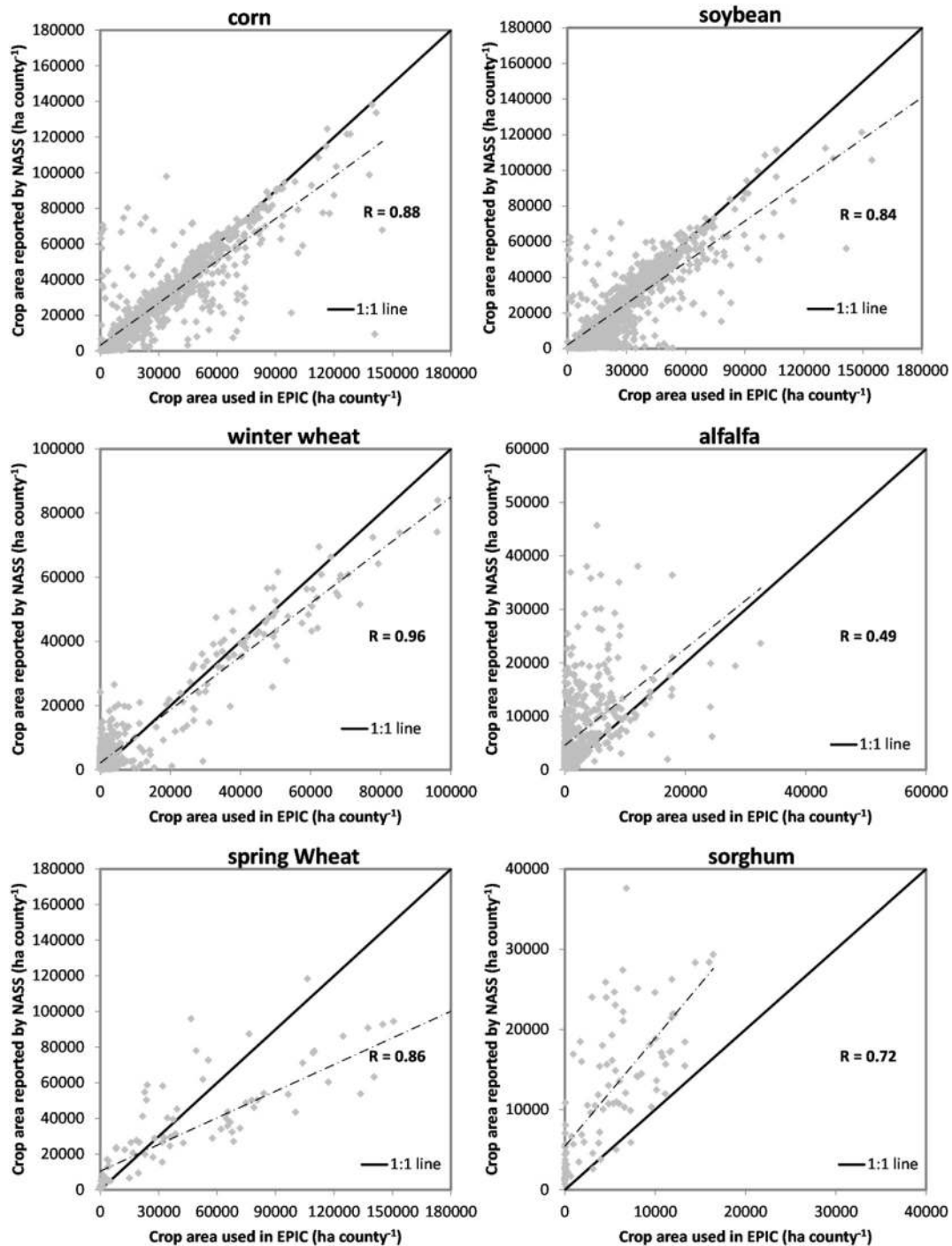
Fig. 12. Spatial correlation between simulated and NASS reported multi-year average (2000–2008) species-specific cropland area.

Due to the lack of regional scale SOC observations, it is difficult to derive solid conclusions about which method performs better under what conditions. Systematic analysis of the sources of uncertainty for each approach is required to better understand their strength and limitations.

3.4.3. Potential parameterization strategies to further improve EPIC simulations

In this modeling exercise, we used *priori* literature reported parameter values and extensive geospatial data to drive EPIC. This model setup method heavily relies on the quality of input data. In Sections 3.4.1 and 3.4.2, we discussed the uncertainties of EPIC simulations related input data. With further improvement in CDL, a more complete SSURGO map and soil properties database, and improved crop management survey data, the reliability of EPIC simulations is expected to be further enhanced. For example, by including more rotations into agricultural landscapes, the accuracy of the crop rotation map can be further improved (Sahajpal et al., 2014). However, this benefit comes at a significant cost of computational resources.

Another popular parameterization strategy consists of identifying the most uncertain parameters and adjusting them within
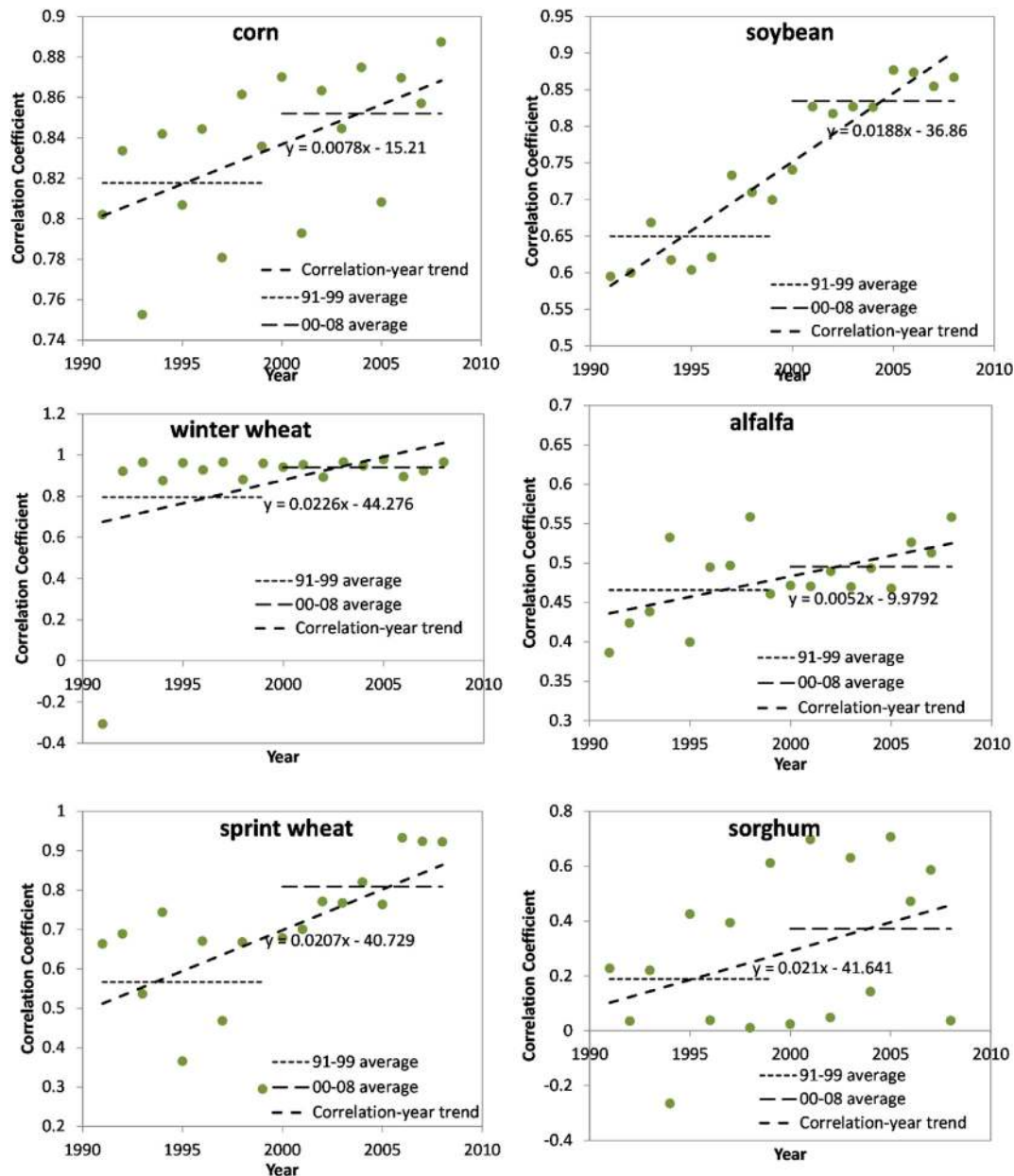
Fig. 13. Time series of annual spatial correlation between simulated and NASS reported species-specific cropland area over 1991–2008.

prescribed ranges to minimize the difference between simulated and observed variables of interest. However, information contents contained in observed variables may not be adequate for characterizing complex hydrologic, biophysical, and biogeochemical processes (Jakeman and Hornberger, 1993). Using crop yields alone to calibrate EPIC may result in parameter overfitting. That is, parameters may be adjusted to compensate for errors associated with input data, model structure, and observations against which a model is calibrated (Jakeman et al., 2006; Zhang et al., 2009). In addition, this strategy often requires running models repeatedly, demanding many more computational resources than the first strategy. Given the limited availability of computing time and data storage capacity, we did not perform extensive parameter calibration in this exercise. Note that uncertainty identification and characterization of input data and model parameters are important, and have the potential to help quantitatively assess errors associated with prediction of C budget components, which are critical for minimizing risks of C related management arrangements and policy making (Post et al., 2008a, 2008b; Updegraff et al., 2010; Varella et al., 2010).

3.4.4. Flexibility of the geospatial modeling framework

As shown in Fig. 2, GAMS encompasses three loosely connected components, each of which can be adapted for other models and analyses. For example, with minor/moderate revisions, the GIS analysis and parallel computing functions can be applied to geospatial data at a global scale or other biophysical and biogeochemical models. If the historical climate databases are replaced with future climate predictions, GAMS can be applied to simulate and understand climate change impacts on agroecosystem productivity (Izaurralde et al., 2003; Thomson et al., 2005a). The composite geospatial layer used to define HSMUs for EPIC simulations contains multi-dimensional information, allowing the integration of the model results with hydrologic and social-economic

models to explore the broader impacts of shifts in agricultural management practices. For example, the hydrologic layer embedded in HSMUs enables the joint use of EPIC land simulations with aquatic processes simulated in watershed models, such as SWAT, to understand water quality consequences of upland soil management.

The geo-location information contained in the composite HSMU layer also allows the spatially modeling results to be aggregated to coarser scales (e.g. low vs. high productive lands within a county, hydrologic unit, or state) that are commensurate with economic and policy analysis models. For example, EPIC simulations at a multi-county scale have been fed into a regionally focused Global Climate Assessment Model (GCAM) for understanding future agricultural land use changes under alternative C prices and radiative forcing levels (Thomson et al., 2013). EPIC simulations were also grouped by differentiating less productive and fertile lands within a 10-digit hydrologic unit and used to explore availability of alternative bioenergy crops under various biomass prices and associated environmental consequences (Egbendewe-Mondzozo et al., 2011, 2013; Gelfand et al., 2013). GAMS provides detailed spatial results for the historical baseline scenario that are critical for robust estimation of benefits and costs of alternative land use scenarios. The flexibility of the geospatial modeling framework makes it easy to provide the inputs required by those socio-economic models and provides opportunities for understanding potential uncertainty arising from aggregating spatial variability.

4. Conclusions

This study introduces a novel geospatial agricultural modeling system, or GAMS, integrating a mechanistic model (in this case EPIC), spatially-resolved data, surveyed management data, and supercomputing functions. Importantly, GAMS was designed to be highly modularized and thus flexible, rendering it straightforward to update input data with emerging observations; replace EPIC with other models; and integrate its simulation results with socio-economic and watershed models—thus making it cost-effective to maintain and adapt GAMS for diverse application purposes.

The overall agreement between the GAMS simulated and inventory estimated cropland county-scale C budgets provided independent confirmation of the credibility of both methods. However, we also detected notable differences in the magnitude of NPP and NEE, as well as in the spatial pattern of SOC change. With individual plant species analyses and annual-scale comparisons, we explored potential causes of the discrepancies by analyzing the differences between EPIC and the inventory method in data requirements, representation of agroecosystem processes, completeness and accuracy of crop management data, and accuracy of spatial crop area representation. Based on these analyses, we discussed strategies to further improve GAMS' performance by updating input data (such as land use, soil, and irrigation) and by designing more efficient parallel computing capability that allows for a systematic examination of uncertainty factors. Improvements will increase our ability to use GAMS to predict C budget components, and understand potential outcomes and risks of C-related management and policy making.

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