

RESEARCH ARTICLE

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Key Points:

- Simulated crop yields from CLM4.5 are validated for the first time at the county level over CONUS
- An optimized fertilization scheme is incorporated into CLM4.5
- Better representations of fertilization and irrigation improve crop yield simulations in CLM4.5

Supporting Information:

- Supporting Information S1

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Simulating county-level crop yields in the Conterminous United States using the Community Land Model: The effects of optimizing irrigation and fertilization

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Abstract In this study, we applied version 4.5 of the Community Land Model (CLM) at a 0.125° resolution to provide the first county-scale model validation for simulating crop yields over the Conterminous United States (CONUS). Large bias was found in simulating crop yields against U.S. Department of Agriculture (USDA) survey data, with county-level root-mean-square error (RMSE) of 42% and 38% for simulated US mean corn and soybean yields, respectively. We then synthesized crop yield, irrigation and fertilization data sets from USDA and U.S. Geological Survey (USGS) to constrain model simulations. Compared with fertilization, irrigation has limited effects on crop yields with improvements limited to irrigated regions. In most current-generation Earth system models (ESMs), fertilizers are applied spatially uniformly with fixed amounts and timing without considering crop fertilizer demand. To address this weakness, we propose a prognostic fertilization scheme that dynamically determines the timing and rate of each fertilizer application, with the annual amounts and valid fertilization time windows constrained by surveyed data. The optimized fertilization scheme reduces RMSE to 22% and 21% of the US mean corn and soybean yields, respectively. Compared with the default CLM4.5, our fertilization scheme substantially improves crop yield simulations especially over major crop growing regions. However, to compensate for the widely documented biases in denitrification rates simulated by CLM4.5, the dynamically determined fertilization timing and rates do not match the fertilization practices of farmers exactly. Therefore, caution should be exercised when extending this method beyond the contemporary conditions.

1. Introduction

Climate variability and change, an important global issue in the context of global warming, has been recognized as a major factor influencing crop production [Schlenker and Roberts, 2009; Lobell et al., 2011; Rosenzweig et al., 2014]. Ray et al. [2015] found that a third of the global agricultural yield variability can be explained by the growing-season climate variability. In addition to changes in mean climate, those in extreme climate have been increasingly reported [Coutou and Robinson, 2013; Christidis et al., 2015; Leng et al., 2015a]. Numerous studies examining the role of climate change in crop yield and production [Rosenzweig et al., 2014] have emphasized the negative impacts from increasing climate extremes such as droughts [Hlavinka et al., 2009; Lobell et al., 2014] and heat waves [Battisti and Naylor, 2009; Lobell et al., 2012; Deryng et al., 2014; Siebert et al., 2014].

In a given climate and agricultural region, food productivity is strongly controlled by irrigation [Postel, 1999; Gleick, 2002; Grassini et al., 2009] and fertilizer application [Stewart et al., 2005; Egli, 2008], both of which are effective adaptation measures to managing the impacts of adverse environmental conditions. In regions receiving insufficient rainfall or experiencing large subseasonal variability of rainfall, irrigation is applied to mitigate water stress on crop growth and production. During the past 40 years, global irrigated land area has expanded from 138 million ha to 277 million ha [Food and Agriculture Organization of the United Nations, 2002]. Irrigated agriculture practiced on ~20% of global agricultural croplands contributes to ~40% of the world's food production [Siebert and Döll, 2010]. In the US, ~17% of cultivated cropland is irrigated, contributing to nearly 50% of total US revenues from agriculture [USDA, 2010]. In addition to water, nutrients are also important for optimum growth of crops. Numerous long-term studies have demonstrated the contributions of fertilizer to the historical increase of crop yields. Stewart et al. [2005] reviewed data representing

362 seasons of crop production and reported that a decline of 40% in wheat yield is expected without regular N and P additions; in extreme cases, 62% of the grain yield was attributable to fertilizer application in Missouri and Kansas. Overall, the US average maize yields would decline by 41%, rice 37%, barley 19%, and wheat 16% in the absence of nitrogen fertilization [Stewart *et al.*, 2005]. The combined effects of climate, irrigation, and fertilizer may account for 60–80% of global yield variability for most major crops [Mueller *et al.*, 2012].

Earth system models (ESMs) such as the Community Land Model (CLM) are effective tools for investigating the water-energy-food systems interactions under climate change. However, agricultural management practices (e.g., irrigation and fertilization) have only recently been included in ESMs [Levis *et al.*, 2012; Drewniak *et al.*, 2013; Leng *et al.*, 2015b; Cai *et al.*, 2016], by applying spatially uniform amounts of fertilizer at fixed rates over croplands [Drewniak *et al.*, 2013; Cai *et al.*, 2016]. Specifically, in CLM4.5, a constant rate of fertilizer is prescribed to the soil mineral pool for 20 days. This scheme has greatly improved CLM crop simulations but does not include the spatial variability of fertilizer applications, and the dynamics between fertilizer demand and supply. In practice, however, plants need different nutrient inputs at different growth stages and at different locations. Applying fertilizers at the wrong time and rates might result in nutrient losses, waste of fertilizer and even damage to the crops and environment [Ju *et al.*, 2009].

In this study, we aim to answer the following questions: (1) how does CLM4.5 perform in simulating crop (i.e., corn and soybean) yields compared to the census data at the county level? (2) Can better representations of agricultural management practices such as fertilization and irrigation improve CLM4.5 crop yield simulations? (3) How important is representing irrigation effect, a factor not considered in previous CLM-based crop modeling studies [Levis *et al.*, 2012; Drewniak *et al.*, 2013; Bilonis *et al.*, 2015], to modeling crop yield in different regions? To answer these questions, we applied CLM4.5 at a high resolution (i.e., 0.125°) to provide the first validation of corn and soybean yield simulations at the county level against census data over the US. Such an evaluation of CLM at a high resolution is a significant advance over previous studies that conducted model evaluation at spatial resolutions (i.e., >2°) too coarse for decision-making [Levis *et al.*, 2012; Drewniak *et al.*, 2013]. We proposed an optimized fertilization scheme that dynamically determines the timing and rate of each fertilizer application considering nutrient demand, with the annual total amount and the valid time window for fertilizer application constrained by observations. From analysis of model simulations, we identified the model deficiencies and potential ways to improve crop yield simulations in CLM.

2. Data and Methodology

2.1. Model Descriptions

CLM is the land component of the Community Earth System Model (CESM) [Gent *et al.*, 2010; Lawrence *et al.*, 2011]. It can be run in an offline or coupled mode in CESM or with the Weather Research and Forecasting (WRF) model [Leung *et al.*, 2006; Ke *et al.*, 2012; Gao *et al.*, 2014]. In this study, version 4.5 of CLM is used, which represents significant improvements to CLM4 in representing canopy conductance, gross primary production, transpiration, hydrology, snow fraction, soil biogeochemistry, and cropping systems [Oleson *et al.*, 2013].

The crop module in CLM4.5 [Levis *et al.*, 2012; Drewniak *et al.*, 2013] is coupled to comprehensive representations of carbon-nitrogen (CN) cycling processes [Thornton and Zimmerman, 2007; Oleson *et al.*, 2013]. Three major crops including corn, soybean, and temperate cereals are represented as managed crop PFTs in CLM, each with its own soil column to distinguish the carbon and nitrogen pools and crop specific management practices. Temperate cereals including wheat, barley, and rye are treated as summer crops (i.e., spring wheat). Due to the limited availability of crop area data to distinguish winter wheat from spring wheat, we will focus on the corn and soybean yields simulations in this study.

Several plant-specific parameters related to photosynthesis and response to soil water stress are incorporated in the model (supporting information Table S1). Specifically, the water content at saturation (i.e., porosity) is defined as

$$\theta_{sat,i} = (1 - f_{om,i})\theta_{sat,min,i} + f_{om,i}\theta_{sat,om} \quad (1)$$

where $f_{om,i}$ is the soil organic matter fraction for layer i defined as $f_{om,i} = \rho_{om,i} / \rho_{om,max}$, $\rho_{om,i}$ is the organic matter density obtained from the CLM organic matter data set, $\rho_{om,max} = 130 \text{ kg m}^{-3}$ is the assumed

density of pure organic soil, $\theta_{sat,min,i}$ is the porosity of mineral soil, and $\theta_{sat,om} = 0.9$ is the porosity of organic matter. Soil texture used in this study is based on a hybrid of 30 arc sec State Soil Geographic Database [Miller and White, 1998]. The two-layer soil type data are then converted to a composition of clay and sand [Cosby et al., 1984] within each 30 arc sec grid cell and interpolated to 10 vertical layers down to a 3.8 m depth. Soil water influence on stomatal conductance is represented by multiplying the minimum conductance by a soil water stress function β_t , which ranges from one when the soil is wet to near zero when the soil is dry. This is a plant-dependent parameter and is determined by the soil water potential for each soil layer, the plant-specific root distribution and its response to soil water stress as follows:

$$\beta_t = \sum_i w_i r_i \quad (2)$$

where w_i is a plant wilting factor for layer i , which is related to the soil water potential (mm) when stomata are fully closed (φ_c) or fully open (φ_o), respectively (supporting information Table S1). r_i is the fraction of roots in layer i , which depends on the plant-dependent root distribution r_a and r_b . Photosynthesis in C3 plants is based on the model of Farquhar et al. [1980] while photosynthesis in C4 plants is based on the model of Collatz et al. [1992]. Several plant-dependent parameters used in photosynthesis are presented in supporting information Table S1.

The CLM4.5 crop growth phenology and CN cycling processes mainly follow that of the AgrolBIS algorithms [Kucharik, 2003]. Four distinct phases of crop phenology in CLM corresponding to planting, leaf emergence, grain fill, and harvest are determined mainly by the percentage of Growing Degree Days (GDD) required for maturity. Allocation of assimilated carbon follows the phenology phases closely that begin with leaf emergence and end with harvest. Specific allocation of carbon to the crop's leaf, live stem, fine roots, and reproductive pools is calculated according to each distinct phenology stage. Altogether there are 20 state variables for vegetation carbon, and 19 for vegetation nitrogen (http://www.cesm.ucar.edu/models/cesm1.2/clm/CLM45_Tech_Note.pdf). Nitrogen allocation is based on the C:N ratios for leaves, stems, roots, organs, and litter (see supporting information Table S2). The total amount of assimilated carbon is down-regulated when soil nitrogen is inadequate to meet plant demand.

In addition to the fertilization scheme [Drewniak et al., 2013], some other new crop features are incorporated in CLM4.5. Specifically, instead of prescribing N as in CLM4.0 [Levis et al., 2012], CLM4.5 adopts an interactive N algorithm with varying pre-grain and post-grain-development C:N ratios for leaves, stems, and roots. Re-translocation from leaves, stems, and roots is represented to fulfill the nitrogen demand for grain development. Nitrogen fixation process for soybean, which is dependent on soil moisture, nitrogen availability, and plant growth stage, is similar to that in the Soil and Water Assessment Tool model [Neitsch et al., 2005].

2.2. Data Preparation

In CLM, an unmanaged crop is represented in the default list of plant functional types (PFTs) and is treated as a generic C3 grass (PFT_{grass}). In this study, the unmanaged crop PFT is derived from the remotely sensed observations from Moderate Resolution Imaging Spectroradiometer (MODIS) at 0.05° [Ke et al., 2012]. The gridded managed crop area data are obtained from Portmann et al. [2010] (ftp://ftp.rz.uni-frankfurt.de/pub/uni-frankfurt/physische_geographie/hydrologie/public/data/MIRCA2000/harvested_area_grids). This data set provides the global distribution and area of irrigated and nonirrigated crops at 5 arc min. To develop the required input data for the model, the 5 arc min crop area data are first resampled at 0.05° consistent with the MODIS-based unmanaged crop PFT. For each grid, the ratio of a specific crop area (r_i) to the total areas is calculated as:

$$r_i = \frac{A_i}{\sum_i A_i} \quad (3)$$

where A_i is the crop area for crop type i . The managed crop PFT ($PFT_{crop,i}$) is calculated as:

$$PFT_{crop,i} = PFT_{grass} \times r_i \quad (4)$$

That is, at each grid cell, the managed crop PFTs are assigned according to the proportions provided by Portmann et al. [2010], but cannot exceed the fraction of the unmanaged crop PFT given by Ke et al. [2012].

Since we focus on corn and soybean, any remaining crop area (i.e., when the total area for corn and soybean is less than the original unmanaged crop PFT) is treated as the unmanaged crop PFT (PFT'_{grass}) as:

$$PFT'_{grass} = PFT_{grass} - \sum_i PFT_{crop,i} \quad (5)$$

For each year, the U.S. Department of Agriculture (USDA) (http://www.nass.usda.gov/Quick_Stats) reports production area and yields for various crops at the scales of counties, states, and agricultural regions/zones over the US. We compiled the USDA census data from 1983 to 2012 for corn and soybean for each county for our analysis period. We also collected the annual fertilizer application amounts from USDA for each state where available. The USDA crop area data set is used for validating the percentages of crop PFTs as the key input for CLM4.5. The USDA crop yields for year 2000 are used for model calibration because the crop PFT area fractions prescribed as the model input represent the conditions in the year 2000. As for validation, we used the USDA crop yield data for the whole study period (i.e., 1983–2012). The USDA fertilizers application data are used for improving the fertilization scheme, and to constrain the model performance in yield estimates. We used the average fertilizer application rate for the periods of 1998–2002, since the crop area distributions in CLM4.5 represent the conditions in year 2000. The missing value of a given year is replaced by the value from the nearest year. States that have no fertilizer application reports from USDA receive the default total amount in the model (i.e., 168 kg/ha for maize and 28 kg/ha for soybean).

For every five years since 1950, the U.S. Geological Survey (USGS) reported water-use estimates for major water demand sectors including domestic, livestock, and irrigation (<http://water.usgs.gov/watuse/>). The county-level irrigation amounts for year 2000 were used to constrain the parameters in the irrigation module such that the simulated irrigation amounts match the observations at the county scale.

In addition to the county-level data set, we collected field data from the Kellogg Biological Station (KBS) (<http://lter.kbs.msu.edu/>) to validate the model at the site level. The KBS is located in Hickory Corners in Michigan, which belongs to the Northeastern region of the US Corn Belt (42.40N, 85.40W). Detailed records of operational practices in terms of soil preparation, planting, fertilization, pesticide application, and harvest are also collected and reported. Data on fertilization include the date, rate, fertilizer type, and equipment used for each application. The KBS adopts corn-soybean-winter wheat rotations where both corn and soybean are rainfed and planted for only 9 years during the overlapping period of 1989–2012. The observed fertilizers application time/rates and the yields of corn and soybean during 1989–2012 were used in this study.

2.3. Dynamic Irrigation Scheme

Soil water availability is a major determinant of plant growth and crop yield, and it is affected by irrigation amount and frequency. CLM includes an irrigation scheme that depends on the dynamics of soil water content [Leng *et al.*, 2013, 2014, 2015b]. The irrigated and nonirrigated fractions of each crop area are derived from Portmann *et al.* [2010]. Irrigation starts when the available soil moisture is inhibiting crop growth (i.e., $\beta_t < 1$) with concurrent LAI value of greater than 0. The irrigation amounts are determined by aggregating the deficit in available soil moisture content and optimum soil moisture content in the root zone for a given crop. The target soil moisture for soil layer i ($W_{target,i}$) is determined by:

$$W_{target} = F_{irrig} \times W_{sat,i} + (1 - F_{irrig}) \times W_{o,i} \quad (6)$$

where $W_{o,i}$ is the minimum soil moisture content resulting in water stress for crop growth; $W_{sat,i}$ is the saturated soil moisture in that layer; F_{irrig} is a weighting parameter governing the optimum soil moisture that determines the irrigation amount and varies between 0 and 1. The irrigation water withdrawn from local surface water [Leng *et al.*, 2013] and groundwater reservoirs [Leng *et al.*, 2014] is applied directly to the soil surface bypassing the canopy. The irrigation scheme is calibrated to match the simulated irrigation amount with the observed amount at the county level using USGS reported data according to the method by Leng *et al.* [2014].

2.4. Optimized Fertilizer Scheme

Applying fertilizers is essential in crop production and is a part of the solution to adequate and secure food supplies worldwide. However, improper application rates and timing might result in low fertilizers use efficiency and damage to the environment (i.e., contamination of surface and ground water). Hence, it is

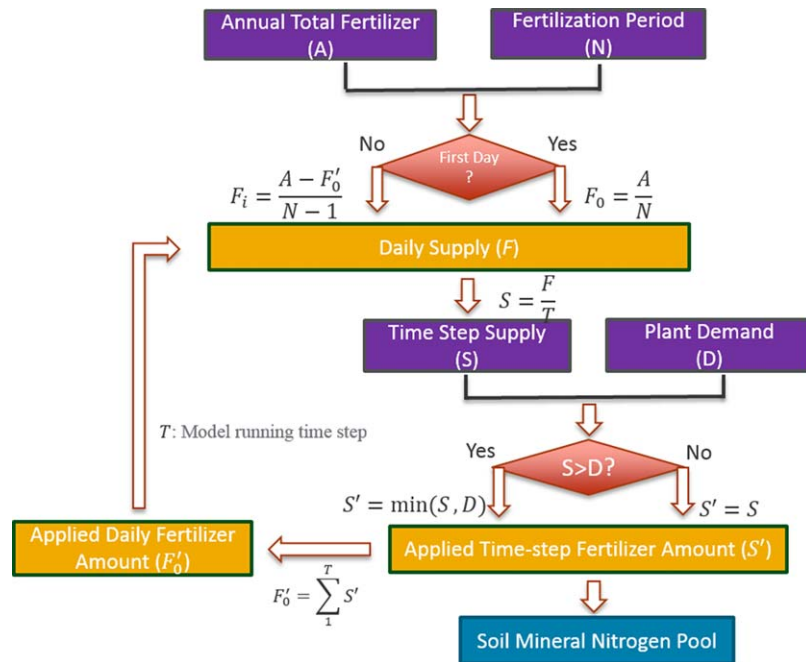


Figure 1. Flowchart of the fertilization scheme proposed in this study.

important to ensure that fertilizers are used responsibly and efficiently. For example, Fertilizer Best Management Practices (BMPs) help ensure production and environmental goals are met through matching of nutrient supply with crop requirements and minimizing nutrient losses from fields [Roberts, 2007]. In this study, we developed and incorporated a fertilizer scheme featuring optimized fertilizer rate and timing, emulating the fertilizer BMPs. Because dates and rates for fertilizer applications are usually determined by farmers' choice, taking into account temperature, precipitation, soil, and other conditions favorable for crop growth, we allowed the model to determine the application date and rate dynamically, by assuming that farmers could find ways to adapt to climate/soil/plant conditions following the guideline of optimizing fertilizer use efficiency.

As illustrated in Figure 1, the starting point is the crop emergence phase, with the fertilizer amount calculated as:

$$F_0 = \frac{A}{N} \quad (7)$$

where A is the total annual fertilizer amount and N is the valid fertilizing periods during which fertilization can occur. The value of A is determined using the USDA reported state level fertilizer use data. In absence of county-level data, we assume that counties within a given state receive the same level of fertilizer amount. N is calibrated by matching the simulated yields with the USDA reported county-level yields. The applied fertilizer amount is then adjusted by

$$F_0' = \min(F_0, D_0) \quad (8)$$

where D_0 is the plant nitrogen uptake demand. The objective function is used to minimize loss and maximize plant uptake. Base on this criterion, there would be no fertilizations when there is no such demand. The fertilizer amount for the second day is then determined by:

$$F_i = \frac{A - F_0'}{N - 1} \quad (9)$$

The above process is iterated until the end of the fertilization period. The standalone crop land unit in the CLM subgrid spatial structure ensures that natural vegetation will not access the fertilizer applied to crops. In the new scheme, the total amount is constrained by observations from USDA reported data at the state

Table 1. Description of the Numerical Experiments

Name	Crop Types	Fertilization	Irrigation
GRASS	No	No	No
CROP_DLFT	Yes	Yes (default)	No
CROP_IRR	Yes	Yes (default)	Yes (optimized)
CROP_OPT	Yes	Yes (optimized)	Yes (optimized)

level. With equations (6) and (7), the daily fertilizer application amount is dynamically determined depending on the supply and demand while the valid fertilization period is obtained through calibration, thus optimizing the efficiency of fertilizer use during the crop growth period.

2.5. Experimental Design

Before the real simulations, a model spin-up procedure was first used by running the model offline with C:N cycling active and using meteorological forcing data obtained from the North American Land Data Assimilation System (NLDAS) [Cosgrove *et al.*, 2003]. The spatial and temporal resolutions of the meteorological data are $0.125^\circ \times 0.125^\circ$ and hourly, respectively, for the period of 1979–2012. The meteorological data included solar radiation, air temperature, air humidity, air pressure, wind speed, and precipitation. We recycled the forcing data for 1300 years to ensure that the C and N pools reached an equilibrium state [Huntzinger *et al.*, 2013]. The resulting state variables from the spin-up period were then interpolated and used to initialize subsequent simulations.

We then performed a series of sensitivity experiments for identifying the sensitive processes and calibrating the parameters of the irrigation and fertilization schemes. Specifically, we perturbed the key parameters governing the simulations of irrigation amount (F_{irrig}) and crop yield (N) following the method of Leng *et al.* [2014]. These sensitivity simulations were conducted for the year 2000, because the crop distribution map for the model represents the condition for that year, and the annual fertilizer amount from USDA is not readily available for the whole period over US. The optimal parameter for each county was selected with the simulated irrigation amount and crop yield matching best the USGS irrigation amount, and USDA crop yield (i.e., the smallest absolute bias), respectively.

In addition, four numerical experiments were conducted (see Table 1) and used in our analysis. The first four years (i.e., 1979–1982) of simulations are excluded in our analysis (i.e., the analysis period is 1983–2012) to account for the effects of initial conditions. The first numerical experiment is a simulation without managed crop (referred to as GRASS) in which crop is treated as C3 grass. The second is the same as GRASS but with managed crop areas and crop specific biogeochemistry cycle active (referred to as CROP_DLFT). The CROP_DLFT adopts the default list of parameters of CLM4.5 such as the C:N ratios during the crop growth stages. Irrigation is not considered in CROP_DLFT for comparison with the study by Drewniak *et al.* [2013] in which CLM was run at the resolution of $2.8^\circ \times 2.8^\circ$. That is, corn and soybean are treated as rain-fed. The third experiment is the same as CROP_DLFT except with irrigation scheme activated (referred to as CROP_IRR). The irrigation application is unique in its dynamic features, and the irrigation amounts are calibrated against USGS reported data. The fourth experiment is the same as CROP_IRR, but includes the optimized fertilization scheme (referred to as CROP_OPT). The fertilizer scheme is unique in that it is optimized for the rate and timing of application, and the annual total amount is constrained by USDA reported data at the state level (Table 2). The difference between CROP_IRR and CROP_DLFT represents the effects of irrigation on crop yields while the difference between CROP_OPT and CROP_DLFT represents the combined benefits of both optimized irrigation and fertilizer application.

3. Results

3.1. Crop Distributions Over US

Figure 2 shows the distribution of fractions (%) of corn and soybean area prescribed in the model and those from the USDA census for the conterminous US at the county level. Most corn growing area is located in

Table 2. Comparison of the Proposed Fertilization Scheme and the Default Treatment in CLM4.5

	Default	Optimized
Annual fertilization amount	Spatially uniform	Spatially variable (from USDA census)
Fertilization period	Spatially uniform (20 days)	Spatially variable (optimized)
Application times	Spatially uniform	Spatially variable and dynamically determined
Rate for each application	Constant	Spatially variable and dynamically determined
Fertilizer use efficiency	Low	High

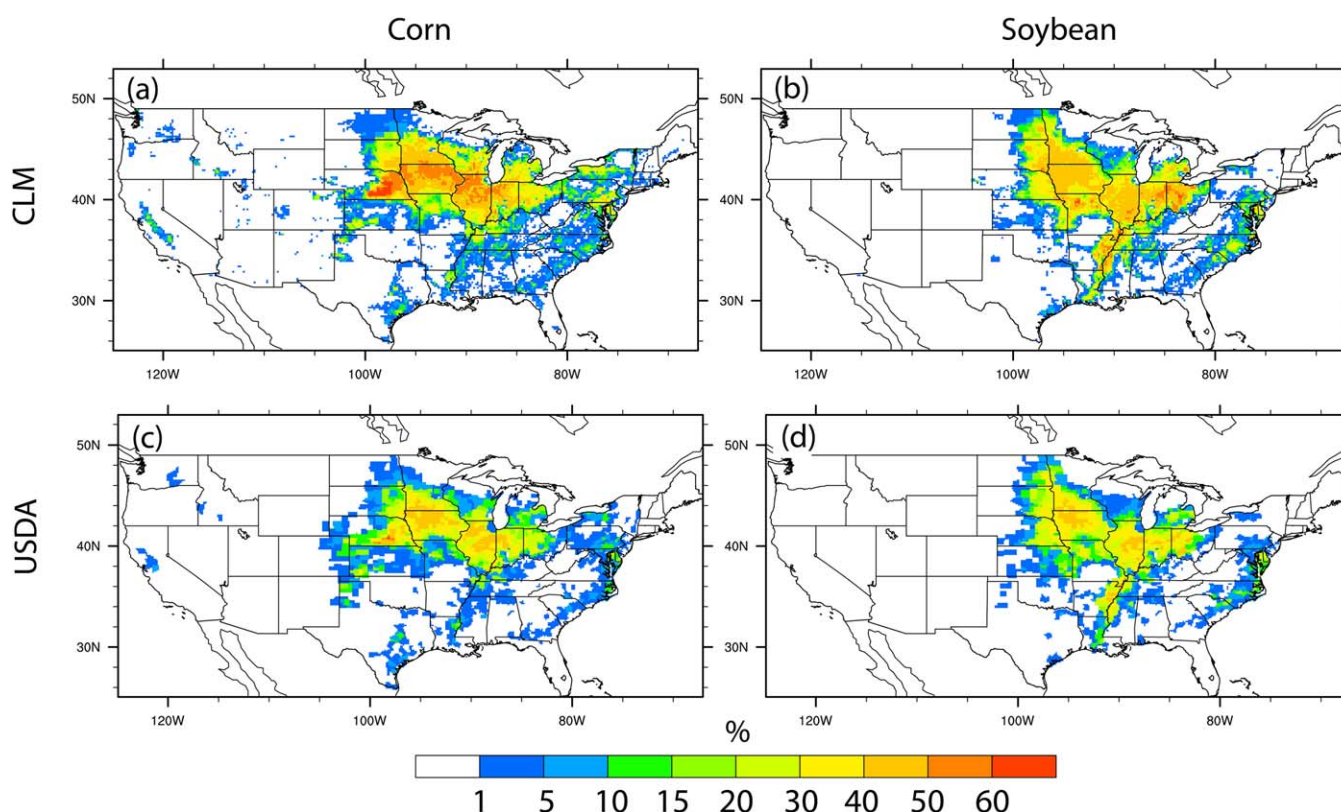


Figure 2. Spatial distribution of the crop growing area percentage relative to the grid area. Figures 2a and 2b are used as inputs for the CLM4.5 while Figures 2c and 2d are based on the USDA census data. Note: Grids within a county are assigned the same value since USDA data are available at the county level.

the major corn belt states (e.g., Iowa, Illinois, Indiana, Ohio, Nebraska, Kansas, Minnesota, and Missouri) which account for 85% of the national harvested corn area. For soybean, the states of Illinois, Iowa, Indiana, Minnesota, Nebraska, Missouri, Ohio, and Arkansas account for 81% of the total national harvested area. The general spatial patterns of corn and soybean area fractions used by the model match well with the USDA data, but with overestimation in the major growing regions. Since the derived cropland fractions are determined based on two different data products, uncertainties arising from the two sources could lead to inevitable bias in modeling the crops using CLM4.5 at the county level, especially for the Western US.

3.2. Irrigation Calibration and Fertilizer Application Optimization

As models evolve through the addition of new processes and improvement of existing algorithms, a given model may not capture all processes well. This is true for irrigation modeling using CLM with explicit representation of crops. Hence, the optimal parameters determined for earlier versions (i.e., CLM4) without differentiation of crop types (i.e., using a generic crop) may not be applicable in the current modeling framework with CLM4.5 that considers crop physiology and phenology, as well as the coupled carbon-nitrogen cycle. Figure 3 shows the simulated irrigation amounts using the calibrated parameter values from CLM4 [i.e., *Leng et al.*, 2014] and those from calibration method described earlier for this study against the USGS reported data. The default parameters from *Leng et al.* [2014] overestimated irrigation amounts in major irrigated areas over the Western, Central, and Southeastern US when compared with the USGS data. After calibrating the new model, the performance was significantly improved for both spatial pattern and magnitude of the irrigation amounts. This also demonstrates that specific crop PFTs might have different impacts on soil hydrology and water demands during the crop growing stages.

Figure 4 shows the distribution of USDA reported annual fertilizer application amounts that were used for constraining the new fertilization scheme. Large spatial variations were found in the major corn growing states, ranging from 80 to 180 kg/ha. Corn in Illinois, Missouri, Ohio, and Kentucky received more than 170 kg/ha fertilizer, while less than 100 kg/ha of fertilizer was applied in Pennsylvania and Mississippi. For

Irrigation Amounts

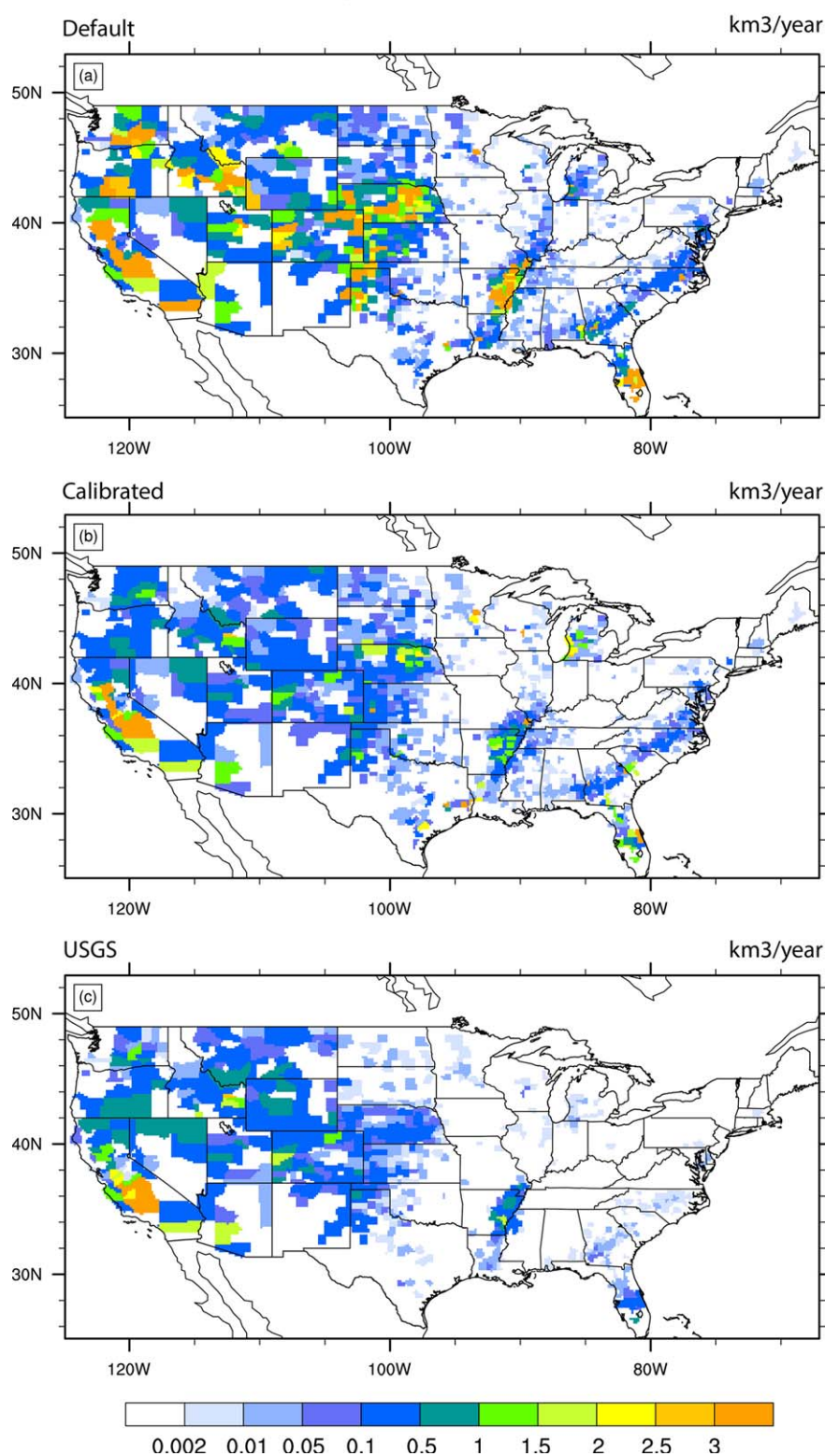


Figure 3. Spatial distribution of the county-level irrigation amounts from CLM4.5 (a) before calibration and (b) after calibration and (c) the USGS data for year 2000 period.

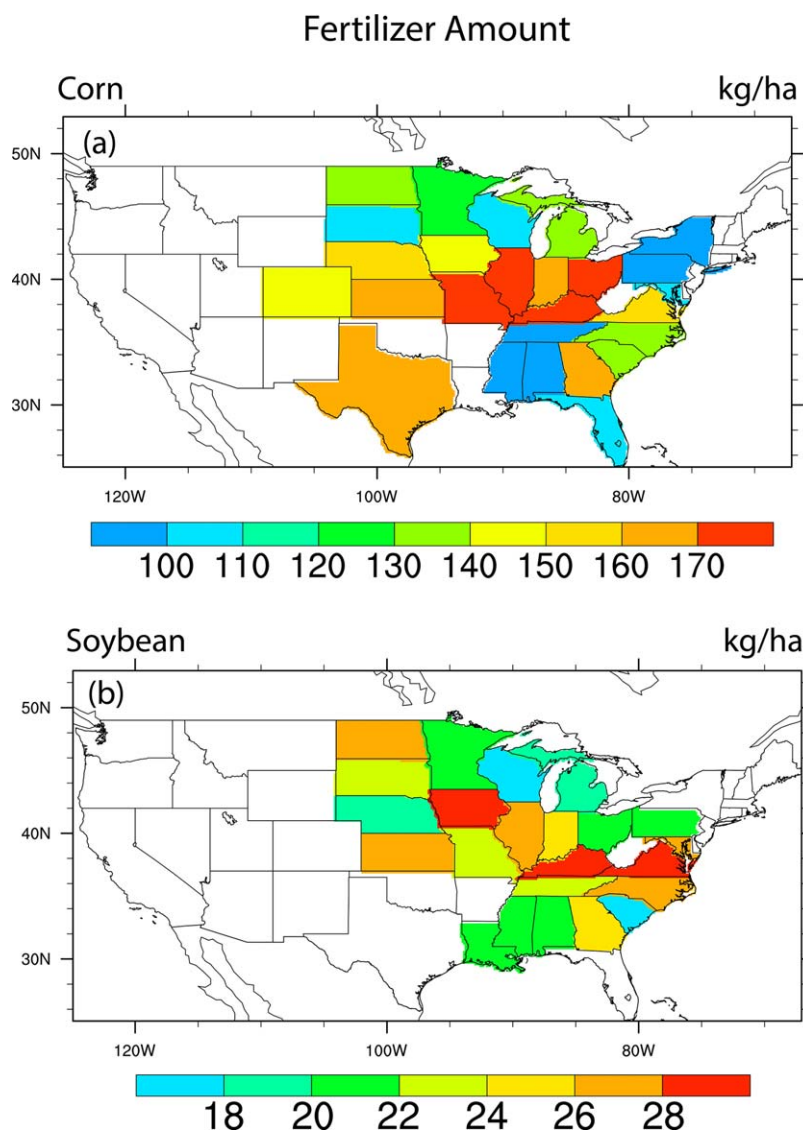


Figure 4. Spatial distributions of the USDA state-level annual fertilizer application amounts for (a) corn and (b) soybean, which are used for constraining the model simulations. Note that counties within a state receive the same fertilization rate. We use a default fertilizer application constant amount for states without reported data.

soybean, the states receiving the highest amounts of fertilizer include Iowa, Kentucky, and Arkansas, while South Carolina, Wisconsin, and Nebraska applied the lowest amounts of fertilizer. Compared with corn, the amount of fertilizer applied to soybean is much lower with the highest amount being about 45 kg/ha. However, the range of soybean fertilizer application rates among the states across US is as wide as 28 kg/ha, which is even larger than the average US soybean fertilization level of 25 kg/ha. The substantial spatial variability in fertilizer application for both corn and soybean clearly suggests that applying fertilizer uniformly across the US as parameterized in the default CLM fertilization module is inappropriate, and highlights the need for representing the spatial variability of fertilization in the model. The proposed fertilization scheme addresses this limitation.

For a given amount of fertilizer, the timing of its applications could have pronounced impact on crop yields as indicated by our sensitivity analyses. Figures 5a and 5b show the spatial distribution of the optimal fertilizer application time windows (i.e., N in equation (7)) for corn and soybean, respectively, at the county level. The optimized fertilizer application time window was determined by matching the county-level crop yields simulated by the model with the corresponding USDA survey data. For corn, long fertilizer application time

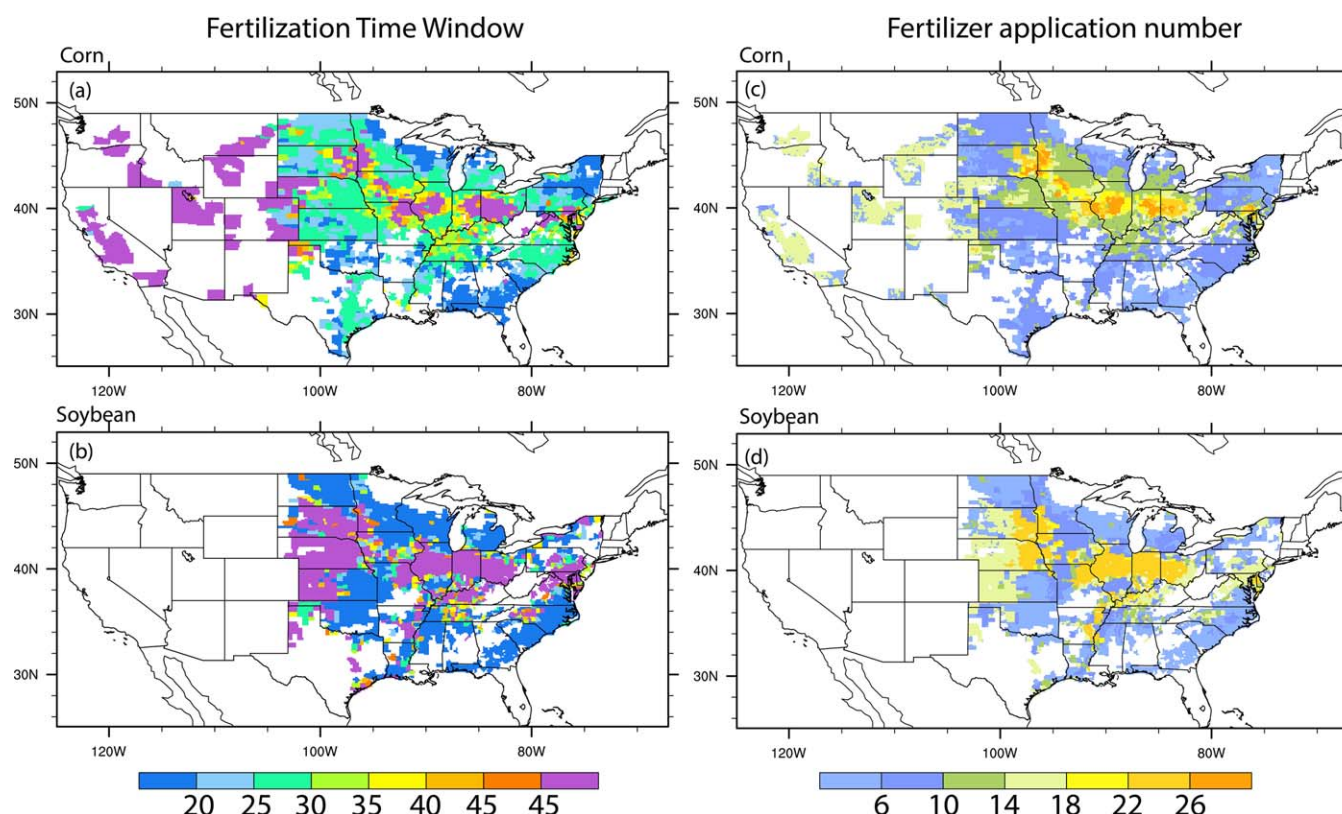


Figure 5. Spatial distributions of the county-level (a, b) valid time windows (days) when fertilizer applications can occur and (c, d) numbers of fertilizer application within the time window for corn and soybean used in the model simulations. Note: Counties with less than 2% of crop area in the model were masked out.

window is required for the West and Central parts of US such as Illinois, Indiana, and Ohio while shorter fertilizer application time window is sufficient for South and Southeast agricultural regions. The fertilizer application time window for soybean is longer than 45 days in South Dakota, Nebraska, Kansas, Illinois, Indiana, and Ohio, while most of the remaining soybean growing regions require a fertilizer application time window of less than 20 days. This suggests that the sensitivity of crop yield to fertilizer application varies across states and counties. In order to capture and represent this factor in CLM4.5 and possibly other models, a spatially distributed fertilizer application approach is required. Note that the optimal fertilization time window refers to the valid time period during which fertilizer could be applied. However, no fertilizer would be applied on specific days when there is no fertilizer demand from the crops since timing and rate of each fertilization are dynamically determined based on the demand by crops (Figure 1). The actual numbers of fertilizer applications for corn and soybean within the valid time window are summarized in Figures 5c and 5d, respectively. The pattern of applications generally follows that of the valid time window with higher application numbers in the Midwest than in other regions. It is evident that our dynamical approach leads to discrepancy in simulated and actual fertilizer application numbers due to model structure deficiency and incomplete knowledge and representation of N dynamics (see the discussions in section 4 for detail). Therefore, improving N parameterizations in CLM has been identified as a topic of high priority in recent CLM developments. We will re-evaluate and the effect of N parameterization on crop modeling and the proposed fertilization scheme once a more recent CLM version (e.g., CLM5) becomes available.

3.3. Comparison of Simulated Crop Yields With USDA Reported Data

Figure 6 shows the county-level corn yields reported by USDA and simulated for the CROP_DFLT, CROP_IRR, and CROP_OPT scenarios across CONUS. Clearly, the default model parameterization significantly underestimated corn yields especially over the Midwest (Figure 6b) compared with the USDA data (Figure 6a). This underestimation could be attributed to the unusual high denitrification rates resulting in ~50% loss of the unused nitrogen [Oleson et al., 2013]. This finding based on the simulated corn yields is in general agreement with results reported by Drewniak et al. [2013] who applied CLM at a resolution of 2.8°. When the

Corn Yields

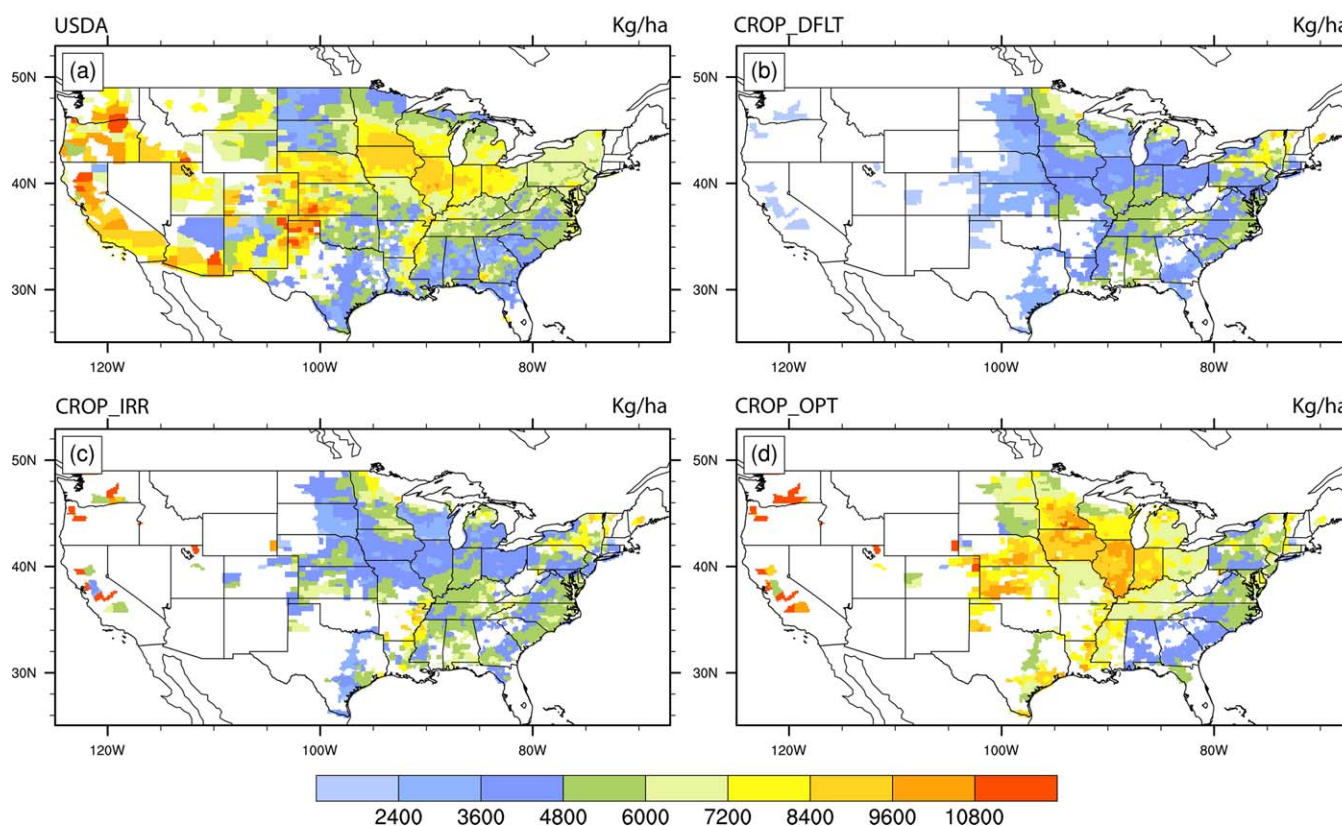


Figure 6. Spatial distributions of the county-level corn yields from (a) USDA data, (b) CROP_DFLT, (c) CROP_IRR, and (d) CROP_OPT simulations.

irrigation scheme was activated, the bias was reduced in regions relying heavily on irrigation for crop growth such as Nebraska, Kansas, and the Western and Southeastern parts of the US. The improved performance with irrigation is limited when looking at the whole US, since only less than 20% of cropland is irrigated [Portmann *et al.*, 2010]. With the optimal fertilization scheme activated, results from the CROP_OPT scenario achieved a better agreement with observations in most corn growing regions. With both irrigation and fertilizer application schemes activated, much of the improvement in model performance occurred over the major corn-belt regions, which contribute to more than 85% of total corn production in the US and constitute $\sim 45\%$ of world trade for both corn and soybean [USDA-ERS, 2016]. The improved performance of CROP_OPT can be largely attributed to the new optimized fertilization scheme (see equations (4–6)) that uses longer fertilization time window and consideration of the dynamics between fertilizer demand and supply, and leads to increased fertilizer use efficiency. For example, in regions such as Illinois, Missouri, Ohio, and Kentucky where similar amounts of annual fertilizer were applied in the default mode (~ 168 kg/ha), the optimized fertilization scheme resulted in much improved crop yield simulations. The effectiveness of increased fertilizer use efficiency is particularly demonstrated in regions receiving lower annual fertilizer amount in the optimized scheme compared with the default mode, mainly because of the consideration of the dynamics between fertilizer demand and supply, thus minimizing the loss of applied fertilizer. Collectively, constraining the annual total fertilizer amount with USDA data, considering the dynamics between fertilizer demand and supply and calibrating the valid fertilizer time window lead to the increase of fertilizer use efficiency and better performance in corn yield simulations.

Unlike corn, soybean can obtain a fraction of its own nitrogen supply through the process of N fixation, which is already represented in the model. A review by Salvagiotti *et al.* [2008] illustrated that there may be a small N deficit between plant demand and the fixed N for soybean yields of ~ 4000 kg/ha, which means that soybean yield would not be restricted by low N supply for yield level of ~ 4000 kg/ha. Furthermore,

Soybean Yields

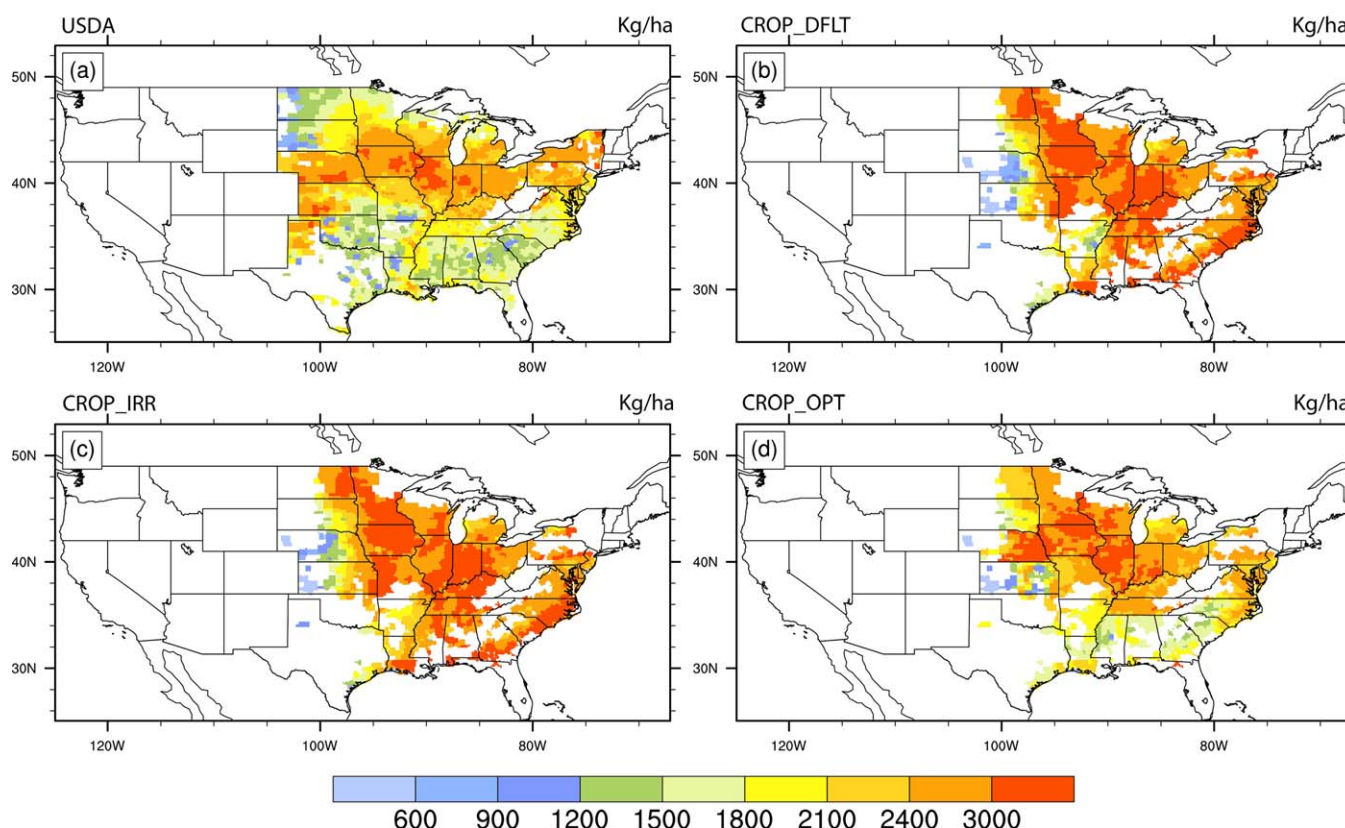


Figure 7. The same as Figure 6, but for soybean.

fertilization could have some impacts on N fixation, thus affecting the net gain in available N to soybean [Salvagiotti *et al.*, 2009]. These studies suggest the importance of proper application of N fertilizer to soybean as the total N amount needed to meet the crop growth demand does vary at different yield levels, while N fertilization interacts with the N fixation. As shown in Figure 7, the CROP_DFLT scenario overestimated soybean yields in most of the soybean growing regions especially in the Midwest and Southeast, but underestimated soybean yields for irrigated areas. The overestimation may be attributed to the improper treatment of fertilizations in the model, ignoring the dynamics between fertilizer demand and supply. With the irrigation scheme activated in CROP_IRR, the underestimation in yield is notably reduced in certain states such as Arkansas while improvement is not evident for other irrigated regions, indicating that water is not a dominant factor for limiting soybean growth in the model. For CROP_OPT, the positive biases were minimized considerably in Iowa, Minnesota, Indiana, Kentucky, and the Southeastern part of US. The reduced positive bias in Iowa, Minnesota, and Indiana was mainly due to the consideration of dynamics between fertilizer demand and supply, given that the total annual fertilizer amount (28 kg/ha) did not change. These results suggest that accounting for dynamics between fertilizer demand and supply is the main reason for better agreement between soybean yield simulations and USDA census data.

Figure 8 shows a scatterplot of the county-level crop yields simulated by the CLM4.5 model and those reported by USDA. Overall, the statistical analyses indicate that the model performance for corn yield simulations was significantly improved as the root-mean-square error (RMSE) decreased from 2843 kg/ha with CROP_DFLT to 1493 kg/ha with CROP_OPT. Meanwhile, the spatial correlation coefficient (R) increased from 0.11 to 0.63, indicating much better performance of the model in capturing spatial variation in crop yields. For soybean, the RMSE decreased from 867 to 462 kg/ha and R increased from 0.29 to 0.68. The bias, however, remains high in terms of the county-level RMSE (~20% of the US mean yield value (Table 3)), mainly due to the poor model performance in the Western US.

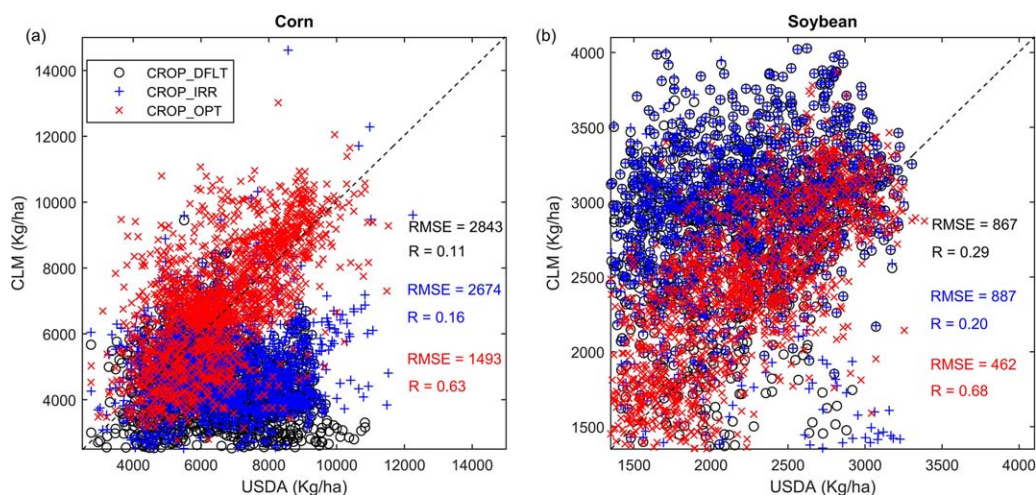


Figure 8. Scatterplot of county-level (a) corn and (b) soybean yields for CROP_DFLT, CROP_IRR, and CROP_OPT simulations as compared with the corresponding USDA data. Since discrepancy exist for location of the crop areas for the model and data (see Figure 2), counties with no crop area identified either by CLM4.5 or USDA are excluded.

When averaged over CONUS (Figure 9a), long-term mean corn yield was underestimated by 2879 kg/ha with CROP_DFLT, or is 38% lower than that the USDA reported yield data. The bias was reduced to -388 kg/ha, or only $\sim 5\%$ lower than the USDA data, after accounting for irrigation and optimized fertilization. Moreover, CROP_OPT captured more interannual variability in corn yield ($R = 0.78$) than CROP_DFLT and CROP_IRR. Bias in soybean yields was reduced from 199 kg/ha for CROP_DFLT to 29 kg/ha for CROP_OPT (Figure 9b). Improvement in capturing the temporal variability of soybean yields was minimal, indicating the existing nitrogen biological fixation algorithm in CLM is likely a key factor controlling the interannual variation of soybean yield instead of fertilizer application variations. This finding is in line with Stewart *et al.* [2005] that eliminating N input to soybeans had minor effects on soybean yields. This result also suggests that responses of different crops to nitrogen fertilizer are crop specific and confounded by other factors such as variable soil fertility and climate conditions.

4. Discussions

4.1. Uncertainty and Limitation of the Proposed Fertilization Scheme

From modeling perspective, where to fertilize (location), when to fertilize (timing), how to fertilize (method), and how much fertilizer (rate) to apply are key aspects of fertilization. Given that fertilization practices vary significantly in different regions, and farmers use different methods to determine the timing and rate of fertilization, and they may or may not act in a consistent manner for lack of information about nutrient availability in the soil due to variations in soil total N, organic matter, and microbial activity, and how much crop N demand is needed due to variations in climatic conditions, soil fertility, pests, etc. [Lobell, 2007], it is

Table 3. Summary of the Model Performance in Simulating the Spatial and Temporal Pattern of Corn and Soybean Yields for 1983–2012 Over US Against USDA Census Data^a

Experiments		Spatial Pattern		Temporal Pattern	
		RMSE	R	Bias	R
CROP_DFLT	Corn	2843 (42%)	0.11	-2879 (-38%)	0.56
	Soybean	867 (38%)	0.29	199 (9%)	0.81
CROP_IRR	Corn	2674 (39%)	0.16	-2011 (-26%)	0.73
	Soybean	887 (39%)	0.2	245 (-11%)	0.82
CROP_OPT	Corn	1493 (22%)	0.63	-388 (-5%)	0.78
	Soybean	462 (21%)	0.68	29 (1%)	0.82

^aNote: RMSE indicate the root-mean-square-error for all crop-specific growing counties over US. Bias is for the long-term mean difference between simulations and observations for the whole US. R is used to indicate the spatial or temporal correlations between simulations and observations.

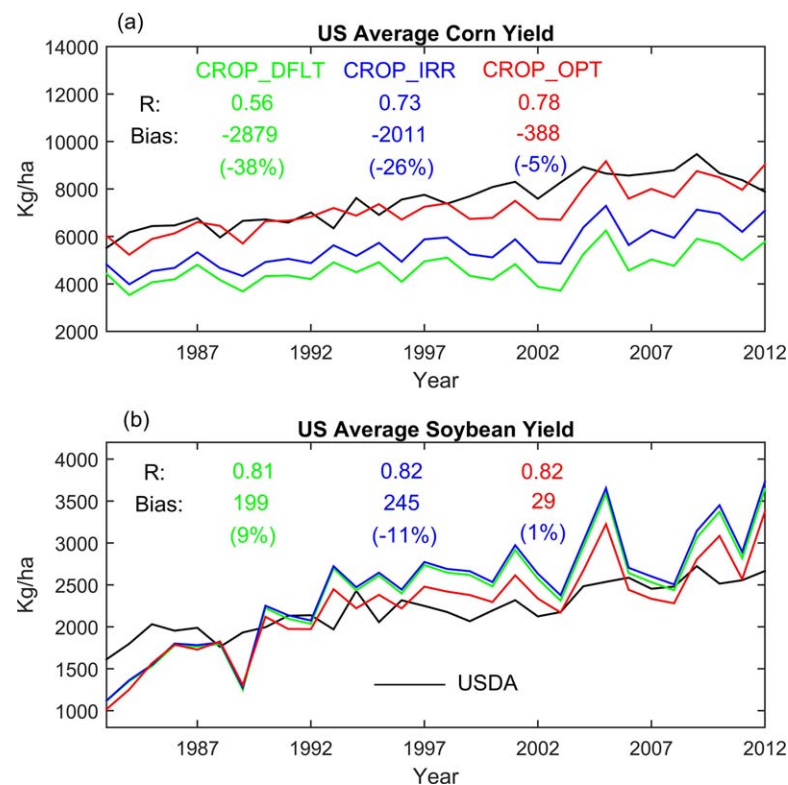


Figure 9. US average (a) corn and (b) soybean yields from USDA (black line), CROP_DFLT (green line), CROP_IRR (blue line), and CROP_OPT (red line) simulations, for the study period 1983–2012.

difficult to represent realistically the actual fertilization practices in large-scale Earth system models. The analysis of USDA reported fertilizer application data revealed a large spatial variability at the regional scale in fertilizer amount used, which further increase the complexity for comparing simulated crop yields with observations. Even at the site-level such as at the KBS, the timing of fertilizer applications varies over the years (Figure 10a). For this location for example, the earliest and latest fertilizer dates (DOY) for corn are 94 and 230, respectively, while they are 129 and 312 for soybean, respectively. Notably, the valid time windows as optimized in this study are consistent with the KBS time window during which fertilizers are applied. Since there are no observations on the exact fertilization timing and rate across the US, both timing and rate for each application have to be treated as internal model parameters. Notably, this is not a unique problem to the study presented here, but rather a common challenge in agro-ecosystem modeling. For example, Zhang *et al.* [2015] used a widely applied agro-ecosystem model (EPIC, Environmental Policy Integrated Climate) in the 12 states in the US Midwest, and discovered that the lack of detailed fertilization information is a key uncertainty in agro-ecosystem models simulation results.

The proposed fertilization approach optimizes the fertilizer use efficiency, which is what farmers pursue in practices and could be achieved by applying slow-releasing fertilizers. Since there are no observations on either the exact fertilization timing and rate, or the actual releasing timing/rates of different types of fertilizers, the application timing and rates are treated as model internal parameters, which is a compromise given the lack of data and limitations in the current model structure. Nevertheless, the fertilization location and annual total amounts are available at the state level in the US. Such data can be used in models such as CLM to better represent agricultural management practices, and constrain the model simulation results and associated uncertainties.

It is imperative to note that our dynamical approach may lead to inconsistency in the application times between the model and practice of the farmers (Figures 5c and 5d). For example, for corn and soybean, there are 1–4 and 1–2 fertilizer applications per year at the KBS during years with available records (Table 4), while the model simulates up to 13 and 9 applications, respectively. Such a discrepancy in fertilization frequency between simulations and observations could be attributed to model structure deficiency in

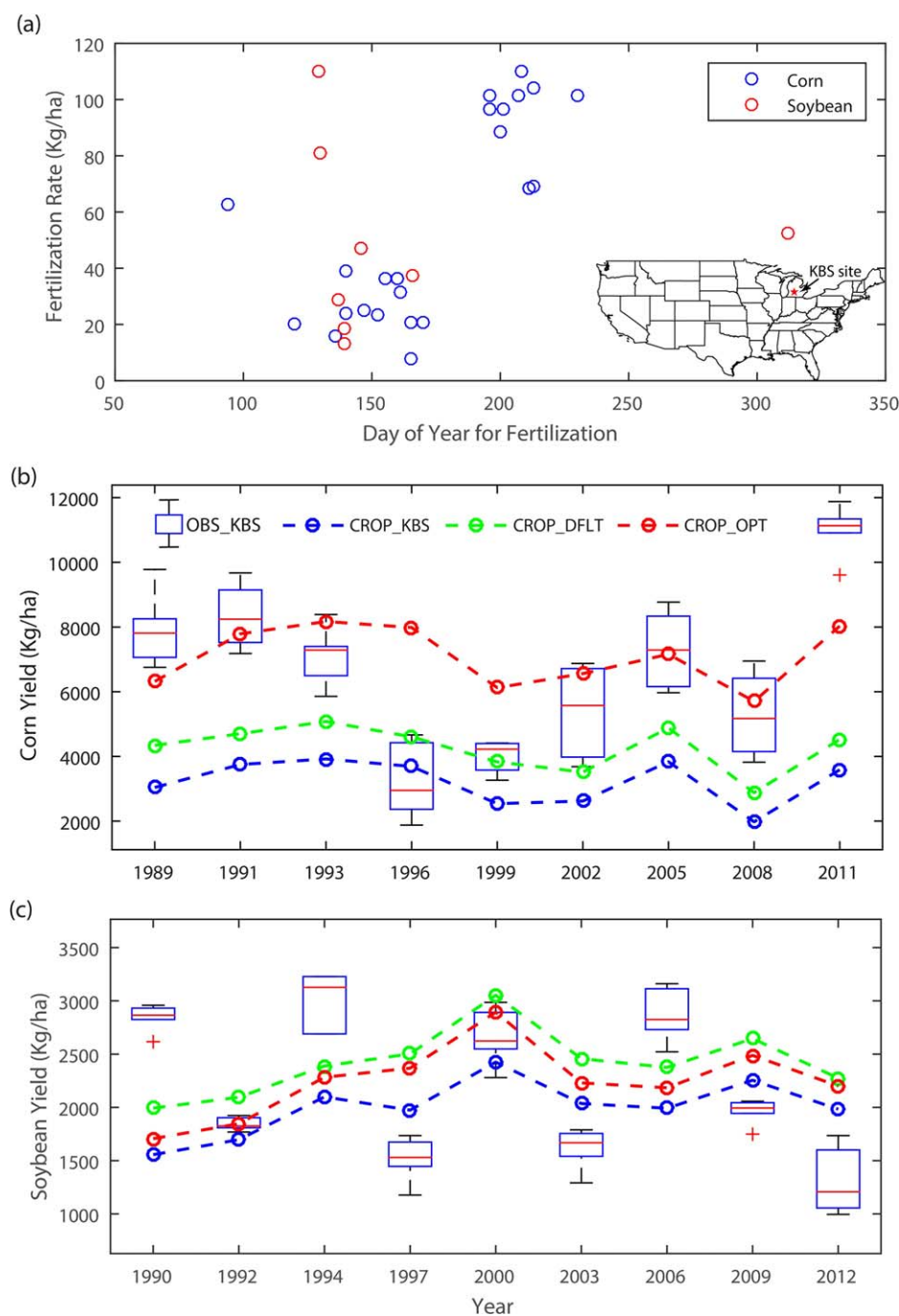


Figure 10. (a) Recorded fertilization timing (Day of Year) and rate for corn and soybean at the Kellogg Biological Station (KBS). Each dot denotes a fertilizer application with the corresponding rate/date for a specific year during 1989–2012. Note: Fertilization records are not available for all years (see Table 4). Figures 10b and 10c are the comparison of simulated corn and soybean yields, respectively, using the recorded fertilization timing/rate (CROP_KBS), default timing/rate (CROP_DFLT) and optimized timing/rate (CROP_OPT) against observed yields (OBS_KBS) at the KBS. Note: Both corn and soybean are planted in only 9 years during 1989–2012, and no irrigation is applied in practice and the numerical experiments. The boxplot is used to show the range of observed crop yields from replicate experiments.

large-scale Earth system models and incomplete knowledge and representation of C:N dynamics. Figures 10b and 10c show the simulated crop yields at the KBS using the recorded rate/timing of each fertilization, the default fertilization treatments, and the proposed approach. Comparing to the observed crop yields, it is evident that a large bias exists in simulating both corn and soybean yields when adopting the observed fertilization rate/timing for KBS. That is, even if we know the exact fertilization rate and timing, the model

Table 4. Summary of Fertilizer Application Numbers at the Kellogg Biological Station (KBS) for the Years With Available Records^a

Corn		Soybean	
Year	Application Number	Year	Application Number
2011	3	2012	2
2008	3	2009	1
2005	3	2006	1
2002	3	2003	2
1999	1	1997	2
1996	4		
1993	3		
1991	2		
1989	1		

^aDetails on the records can be found at <http://kbs.msu.edu/>.

would fail to reproduce N availability in soils, leading to poor model performance despite the inclusion of fertilization timing/rate). Specifically, it has been reported that CLM unrealistically overestimates denitrification when compared to estimates from literature, resulting in a 50% loss of the unused available nitrogen [Nevison *et al.*, 2016]. Houlton *et al.* [2015] demonstrated that CLM4.5 predicted unrealistic frequency and spatial distributions of f_{denit} (proportion of soil nitrogen emissions to denitrification). Zhu and Riley [2015] found that this failure is due primarily to unrealistic assumptions regarding nitrogen competition, and also due to poor numerical representation of advective fluxes. Our results confirm previous findings and suggest that a thorough evaluation and reformulation of the nitrogen scheme in CLM should be performed. Nevertheless, given such a deficiency, the derived fertilization time window and dynamically determined fertilizer timing/rate become effective

measures to compensate for the rapid denitrification in CLM [Drewniak *et al.*, 2013; Tang *et al.*, 2013; Bouskill *et al.*, 2014; Fan *et al.*, 2015; Nevison *et al.*, 2016]. Indeed, compared with the default model treatment, our approach leads to closer agreement at the site, county and country levels in terms of corn yields, although biases still remain for certain years and regions. As CLM continue to evolve, we expect that the N parameterizations could be improved in the newer versions. We will re-evaluate the new parameterizations and their implications to agro-ecosystems in future studies, now that we have a better understanding of the importance of fertilizer and irrigation management practices.

Land management practices, such as irrigation and fertilization, have only recently been included in land surface models [Levis *et al.*, 2012; Drewniak *et al.*, 2013; Leng *et al.*, 2015b; Cai *et al.*, 2016], and great challenges still exist in representing them in Earth system models. In earlier versions of CLM, 20 consecutive days of fertilization were adopted for the whole US independent of crop type and location, while maintaining the fertilizer rate the same within the 20 day time window [Drewniak *et al.*, 2013]. In this study, we attempted to incorporate all available information on irrigation and fertilization management practices into the model and applied fertilization dynamically in time and space. The annual total amount is prescribed based on the USDA census, while the timing and rate for each application during the valid time windows are dynamically determined considering the crop fertilizer demand (Table 2). Indeed, our results show that by synthesizing available observations-based management practices into the model, our fertilization scheme can effectively reduce losses of nitrogen, leading to significant improvement of model performance in crop yield at the regional scale

4.2. Other Sources of Uncertainties and Limitations

In addition to fertilization scheme, other sources of uncertainties due to process understanding and model limitations should be acknowledged. For example, the maximum available water content is determined by the soil texture data set and is prescribed as inputs in the model. However, variations in the maximum available water content can affect the maximum level of irrigation during the calibration process and thus introducing some uncertainties in irrigation amounts and their effects. Nevertheless, we show that irrigation management approach results in a good match with the USGS reported irrigation amount at the county level. Although the gridded crop areas were developed as input to match and constrain model simulations, the gridded crop area data at the county scale still contain, in general, some bias that will propagate into the crop simulations. In addition, uncertainties from the gridded temperature data, among other meteorological forcing data, should also be acknowledged since the Growing Degree Days (GDDs) used for determining the crop development stages is based on daily temperature [Luo *et al.*, 2003]. Further, we did not differentiate the irrigation amounts between crop types since there is no crop-specific irrigation data reported over the conterminous US. Hence, the same calibrated parameter value is used for both corn and soybean within a grid cell. Therefore, more efforts are needed to develop consistent and reliable data sets to better represent the crop-specific area distributions and irrigation amounts, and characterizing the uncertainty in the gridded data at finer spatial scales.

As our understanding of the integrated Earth system evolves, Earth system models and their components (e.g., CLM) are becoming more complex by closely coupling a greater number of processes, resulting in structural uncertainties which to some extent reflect the incomplete knowledge in parameterizing the biogeochemical processes and/or constraining the related parameter values. For example, even though interactive C and N dynamics are explicitly represented in CLM, many aspects of the functioning of the terrestrial N cycle and its interactions with the C cycle, as well as the causes of wide-spread terrestrial N limitation remain poorly understood and therefore are highly parameterized and simplified in these models [Levis *et al.*, 2014; Drewniak *et al.*, 2015]. Developing more mechanistic representations of these processes often requires comprehensive field investigations and/or long-term observations, which are out of the scope of this study; however, we identify a need for a greater focus on these processes in the future for model improvement and evaluation, and uncertainty characterization.

Parameter tuning is a common practice to deal with model uncertainties by optimizing the simulations against observations for improving model predictions [Billionis *et al.*, 2015; Huang *et al.*, 2016]. Specifically, the terrestrial N pools receive inputs from atmospheric deposition and biological N fixation and output N through leaching and gaseous losses, which together determine the long-term terrestrial N balance, and thus N availability. The degree of sensitivity of corn yield response to N fertilization is much greater than that of legumes such as soybeans or peanuts [Stewart *et al.*, 2005], which could be further confounded by many other factors such as variable soil fertility levels and climate conditions. We model fertilization by constraining its total amount against observations while optimizing the timing and application rates in the model. As a consequence, the fertilizers applications may not completely fit those in real practice for some cases, and the information required to evaluate models at this level of spatial and temporal details may not exist. These uncertainties together contribute undoubtedly to biases in the simulated yields in CLM especially in terms of the county-level RMSE. However, incorporating an optimized fertilizer application together with a dynamic irrigation scheme with calibrated parameters constrained by observations results in promising improvements in simulating mean annual crops yields and their variability and spatial distribution, especially for the Midwestern region of US. This highlights the need for proper representations of agricultural management practices in the agro-ecosystem component of Earth system models.

5. Conclusions

Crop yields are affected by many factors such as climate conditions and agricultural management practices. Among these factors, nutrients and water act as limiting factors across major crop growing regions such as the US Great Plains [USDA, 2010; Stewart *et al.*, 2005]. In this study, we evaluated the performance of CLM4.5 in simulating the county-level corn and soybean yields in terms of their spatial pattern, mean and temporal variability, and quantified how the improvements through optimizing two important management practices (i.e., irrigation and fertilization) influence crop yield simulations. In doing so, we developed geospatial data sets on agricultural management practices by synthesizing crop yields, irrigation, and fertilizers application rates reported by USDA and USGS, and incorporated such information into CLM4.5 to investigate the model behaviors and its potential improvements in simulating corn and soybean yields at the county scale across the CONUS.

Our results show that when averaged over the CONUS, the long-term mean bias for simulated corn and soybean yields using the default CLM parameterization is -38% and 9% , respectively, compared with USDA census data. Given the fact that nitrogen availability strongly limits crop productivity, we hypothesized that an improved representation of fertilization could improve model performance. Our numerical experiments suggest that with an optimized fertilization scheme in which fertilizer is applied dynamically and variably in time and space with the annual total amount and the valid time window constrained by USDA census data, CLM captured better the spatial patterns of corn and soybean yields, as well as the interannual variability of corn yields. Much of the model improvement occurred over the Midwest US, or the Corn Belt regions where corn and soybean production account for more than 80% of the national total production. Improvements in capturing the variability of soybean yields are relatively small, which may be attributed to the strength of the existing representation of soybean nitrogen fixation process in the CLM4.5 model. Noticeable biases still exist over the corn growing area in the Western US, mainly due to uncertainty in location and area fractions of crop PFTs used as input to the model.

Explicit representations of agro-ecosystems (i.e., specific crop types and management practices), as opposed to treating crops as natural grasses, were absent in most ESMs used for the latest IPCC report [IPCC, 2013; Ciais *et al.*, 2013]. To address such a limitation, CLM4.5 includes an explicit representation of crops coupled to nitrogen cycling and agricultural management practices. By providing the first validation of CLM4.5 for crop yield simulations at the county level, this study contributes to assessing the model behavior in simulating the spatial and temporal patterns of crop yields, and identifying the model deficiencies and future development directions. Although the benefits of incorporating the proposed fertilizer scheme is evident in reducing biases in crop yield simulations, we acknowledge that the simulated fertilization timing/rates require further improvement given the limited data, difficulties in representing fertilization in ESMs, and the inherent deficiency in model structure with unrealistically high denitrification rates. For example, for corn and soybean, there are 1–4 and 1–2 fertilizer applications per year, respectively, at the KBS based on available records, while the model simulated up to 13 and 9 applications, respectively. Over the CONUS, it is evident that the simulated fertilizer application numbers are biased high, although it is hard to quantify the magnitude and sources of biases due to lack of observations. Thus, caution should be exercised when using such an approach, which is only applicable where and when fertilizer amounts are available. Future efforts should be dedicated to model development, including the agricultural management practices (e.g., fertilization, irrigation, etc.) and biogeochemical processes (e.g., denitrification), to improve CLM's capabilities for simulating more realistically crop production as affected by anthropogenic disturbances, and changes in biogeochemical and hydrological cycles, and climate.

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