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Effects of automatic multi-objective optimization of crop models on corn yield reproducibility in the U.S.A.

Kenichi Tatsumi*

Department of Environmental and Agricultural Engineering, Tokyo University of Agriculture and Technology, 3-5-8 Saiwai-cho, Fuchu 183-8509, Tokyo, Japan

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ABSTRACT

This study presents a detailed analysis relating to the effectiveness and efficiency of the multi-objective complex evolution (MOCOM-UA) algorithm on the reproducibility of corn yield for the period 1999–2010 in the United States of America. The algorithm was coupled with the Environmental Policy Integrated Climate (EPIC) model and is capable of solving the multi-objective calibration problem for crop models. Understanding how model parameters are determined from past research work is especially difficult because parameter determination is usually performed by manual trial and error methods and still remains a black box. Single-objective functions are often inadequate to properly measure all characteristics of the observed datasets and do not usually provide parameter estimates that are considered acceptable. In contrast, a multi-criteria optimization would allow the analysis of the trade-offs among different criteria, and would indicate the limitations of the current crop model structure better. Therefore, a multi-objective algorithm was used in this study to identify the critical model parameters and to glean a better understanding of model uncertainties. The uncertainty analysis of the model was performed by comparing simulation results obtained using randomly generated initial parameters and inputs with the attainable calibrated parameters and inputs. Three model parameters (biomass to energy ratio (BE), harvest index (HI), potential heat units (PHU)) and two inputs (planting dates (PDAY), planting density (PDENS)) were optimized on a grid-scale to capture a more realistic spatial pattern and temporal variability of corn yield. The conclusions derived from this study are: (1) the critical parameters needed to reproduce corn yield with EPIC are BE, HI, and PHU; (2) the MOCOM-UA calibration procedure is highly effective in improving the spatial agreement and temporal variability of corn yield and for reducing the width of the uncertainty band; (3) by using the calibrated parameter sets, measurement errors of spatial-averaged ensemble mean yield are significantly improved; (4) simulation using the EPIC model showed better performance in the major corn area with relatively accurate input datasets, but performed poorly in the minor corn area with lower yield and corn area ratio. This study highlights the projected contribution of the multi-objective optimization procedure in identifying critical model parameters in reducing the width of the uncertainty band, and in improving the spatial agreement and temporal variability of corn yield. Future work should focus on the effect of optimizing more appropriate parameters such as those that affect water availability or soil fertility status on crop yield reproducibility.

1. Introduction

Process-based crop growth models have been developed to evaluate the impact of climate changes on food production and climate adaptation, and to develop strategies such as risk management of pesticide and fertilizer application in the agricultural framework. Over the years, several process-based models have been developed that identify some parameters or inputs that could potentially affect the final crop yield. For example, the APSIM model was developed to simulate the biophysical processes in farming systems, utilizing information on soil, crop, tree, pasture and livestock (Keating et al., 2003). The DAYCENT model, which is the daily time-step version of the CENTURY biogeochemical model, was developed to simulate the long-term response of ecosystems to changes in climate, environmental factors, land use and agricultural management practices (Parton and Rasmussen, 1994; Parton et al., 1998). The EPIC model was mainly developed to assess the effect of soil erosion on productivity in agricultural management (Sharpley

* Tel.: +81 42 367 5679; fax: +81 42 367 5679.
E-mail address: ktatsumi@cc.tuat.ac.jp

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and Williams, 1990). The DSSAT model has been used to assess crop growth performance in response to changes in environmental conditions and farming practices (Keating et al., 2003). Tatsumi et al. (2011) developed the iGAEZ model based on an earlier model developed by Fischer et al. (2002) to simulate the crop yield on a global scale. However, despite the preponderance of such model systems, using any of these existing models for the assessment and detection of crop yield poses several limitations. Different models lead to different results even when using the same input and forcing datasets because of the differences in the model structure. In addition, the setting of model parameters and inputs with respect to factors like weather, soil, fertilizer, crop, and field operation will influence the results and increase or decrease model uncertainties. This source of variability is known as parameter and input uncertainty. The uncertainties associated with current crop models under a wide range of model parameters and inputs remain largely unquantified (Li et al., 2014). Therefore, sufficient knowledge about these uncertainties can provide valuable information to consider during model development and to propose new strategies for sustainable agriculture.

A common approach for determining crop model parameters such as harvest index (HI), biomass to energy ratio (BE), and potential heat units (PHU) that would affect corn productivity or phenology for large-scale crop simulation is to use a manual trial-and-error calibration that is based on model input datasets from representative range of parameter space and to assume that a given area is homogeneous. However, since reliable and accurate input datasets with high resolution are difficult to obtain on weather and soil, especially for larger areas, spatial interpolation of data is frequently carried out as a pre-processing step in crop yield simulation. But in reality, there is a lot of heterogeneity within the grid area (van Ittersum et al., 2013) and this could introduce another uncertainty during crop simulation. Other inputs relating to tillage operation in agricultural land use, planting density (PDENS), planting (PDAY) and harvesting dates, fertilizers and nutrient materials, and crop genotype information have been used sparingly; however, they bring about large uncertainties as well. The determination of these parameters and inputs has widely been performed based on the predominant management practices obtained from literature and from field experiments conducted in the entire study area. Few large-scale crop simulations provide clear information on estimating the uncertainty of the model parameters, inputs and reproducible protocols for adjusting these parameters and inputs are few. Past research so far has not considered spatial heterogeneity in detail, and therefore, does not reflect the region-specific agricultural systems in crop simulation protocols (de Wit et al., 2010; Tatsumi et al., 2011; Waha et al., 2011).

The limited consideration of many important model parameters and inputs has rendered the application of most available crop models to wide areas rather difficult. Therefore it is imperative for a model calibration to closely match the behavior of the real agricultural system it is intended to represent, so that it can genuinely improve the accuracy of the crop yield simulation results and aid in developing better agricultural practices in the region. In order to achieve this, optimizing model parameters and inputs is critical. Optimization allows for explicit interpretation of simulation outputs, but in many scientific studies using crop simulation, the specific determination method and the procedure of model parameters and inputs are not clearly shown (e.g., Brown et al., 2000; Chung et al., 1999; Izaurralde et al., 2003; Ko et al., 2009; Niu et al., 2009). In some studies, a single-objective calibration by manually adjusting the parameters has been conducted at the regional and continental scale (Angulo et al., 2013; Therond et al., 2011; Xiong et al., 2014). However, single-objective functions are often inadequate to properly measure all characteristics of the observed datasets that are deemed important, and do not usually provide parameter estimates that are considered acceptable (Vrugt et al., 2003). In contrast, a multi-criteria optimization would allow the analysis of the trade-offs among different criteria, and would enable the agronomist to perceive the limitations of the current crop model structure better. Recently, Bulatewicz et al. (2009) calibrated ten parameters using a genetic algorithm in irrigated lands of Kansas. However, barring this, only limited work has been carried out on the automatic and multi-objective calibration approach to simulate crop yield in wide areas.

Drawing from the above insights, the present study investigated the usefulness of a multi-objective optimization model for corn yield simulation across the U.S., using the best available planting date and harvest date, and geophysical, geological and meteorological forcing datasets for the period 1999–2010. It is assumed that the optimized grid-based, region-specific parameters and inputs will improve the spatial agreement of crop yield between the simulated and reported yield. Here, I propose a novel approach to optimize the parameters and inputs in the module of the widely used EPIC model using the multi-objective complex evolution (MOCOM-UA) (Yapo et al., 1998) algorithm to achieve a better understanding of the crop yield model structure. The specific objectives of the present study are as follows: (1) to provide a detailed method of the corn yield simulation with currently available datasets that are reliable; (2) to suggest an appropriate and efficient multi-objective optimization approach for improving crop yield simulation results based on limited input datasets; (3) to test the improvement effected by the MOCOM-UA method in reducing the width of the uncertainty band across the U.S.

2. Materials and methods

Crop yield simulation by the EPIC model mainly requires datasets concerning weather, soil, topography, field operation, and crop. These input datasets were collected from different public sources, and each original raster map were resampled to a finer (coarser) simulation grid cells using interpolation (aggregation) method (Table 1). The simulation area and period are 23–50°N and 120–60°W at a $0.25^\circ \times 0.25^\circ$ latitude–longitude spatial resolution from 1999 to 2010.

2.1. Crop model

The EPIC model version 0509 (Sharpley and Williams, 1990; Williams, 1995; Williams et al., 2006) was used to test the effectiveness of the optimization method and reproducibility of corn yield. This model has been widely used to simulate soil carbon sequestration, management practices, nutrient cycling and loss, and climate change impact on crop yield (e.g., Easterling et al., 1998; Ko et al., 2009; Niu et al., 2009; Peruta et al., 2014; Wang et al., 2011; Zhao et al., 2013). This model is an open-source software and has built-in FORTRAN programing language to enable the development and application of the calibration procedure. In recent years, the model has been extended into a comprehensive soil-water-atmosphere-crop-management model simulating crop growth in complex schemes (Williams et al., 2006). The model constitutes nine major components, namely, weather, hydrology, soil erosion, manure, nutrient, pesticide fate, crop growth, tillage machinery, and field operation schedule. The total number of model parameters and inputs is more than 300. In principle, though the model parameters are set with the contextually correct meaning, the coefficients of most miscellaneous parameters have only a model-intrinsic meaning (Peruta et al., 2014). The default value of model parameters can be obtained from the EPIC program package with unique values for each crop, but the values need to be optimized with respect to the circumstances in each study region.

Table 1
Datasets used in this study.

Data set	Name	Original spatial resolution	Resample method	Period	Source
Reported yield	NASS	County-level	Nearest neighbor	1999–2010	USDA (2014a)
Planting and harvesting dates	USDA	State-level	Nearest neighbor	20 years of historical crop progress estimates	USDA (2010)
Meteorological forcing	GMFD[a]	0.25 degree	Not used	1999–2010	Sheffield et al. (2006)
Elevation	GTOPO30	30 arcs	Regularized spline with tension	–	USGS (1996)
Terrain slope	ASTER GDEM	3 arcs	Nearest neighbor	–	Abrams et al. (2010)
Soil type and hydrological properties	HWSD	30 arcs	Mode aggregation (soil type) and Mean aggregation	2000 (the nominal year)	FAO (2012)
Soil albedo	ECOCLIMAP	about 1 km	Mean aggregation	2000	Champeaux et al. (2005), Masson et al. (2003)
Fertilizer and Manure	GFM[b]	0.5 degree	Nearest neighbor	Late 1990s	Potter et al. (2010), SEDAC (2015)
Irrigated and rainfed cultivated area	MIRCA2000	5 arcmin	Sum aggregation	2000	Portmann et al. (2010)

[a] GMFD (global meteorological forcing dataset for land surface modeling).
[b] GFM (Global Fertilizer and Manure, Version 1 Data Collection).

Crop yield in the model is estimated as a function of BE, HI, PDENS, photosynthetic active radiation (PAR), and vapor pressure deficit (VPD), and is reduced through stress factors related to temperature, water, soil and air. The potential biomass is calculated from intercepted PAR and VPD values, and was adjusted to the actual biomass through water, temperature, aeration, and nutrient stress factor values. Each stress factor has a range from 0.0 to 1.0, and will affect the potential crop growth and yield. The actual yield is estimated using a proportion of economic yield over total biomass, which is referred to as the harvest index. Fig. 1 shows the diagram of crop yield simulation framework in the EPIC model. The detailed explanation of EPIC goes beyond the scope of this work, and more technical information on the EPIC can be found in the source code of this model.

2.2. Crop data

In this study, corn crop was selected to test the MOCOM-UA method. The U.S. is the world-leading producer of corn, both in terms of value of production and of acreage of corn grown (FAOSTAT, 2014). The major corn growing area in the U.S. is the so-called "Corn Belt", which mainly includes South Dakota, Nebraska, Minnesota, Iowa, Missouri, Wisconsin, Illinois, Indiana, and Ohio.

Reported corn yields were obtained from USDA National Agricultural Statistics Service (NASS; USDA, 2014a). This service collects data on all commodities produced on U.S. farms and includes planting, harvesting, and yield information, as well as expenses, income, and operator characteristics for agricultural districts, counties, states and the entire nation (USDA, 2014a). For the present study, county-level yearly corn yields for the period 1999–2010 were used for optimizing the selected model parameters and inputs (see Section 2.6.2) and for evaluating model accuracy. The county areas with missing yield reports in that period were removed from the simulation. As a result, a total number of 3457 mesh grids were obtained in the simulation.

2.3. Meteorological forcing data

The simulation by the EPIC model requires six daily meteorological forcing variables (minimum and maximum air temperature at 2-m above ground, precipitation, solar radiation, relative humidity, and wind speed) for the period 1999–2010. These datasets were obtained from a high-resolution global meteorological forcing datasets for land surface modeling (Sheffield et al., 2006). This database was constructed with a geographical resolution of 0.25 degrees by combining a suite of global observation-based datasets with the National Centers for Environmental Prediction/National Centers for Atmospheric Research (NCEP/NCAR) reanalysis.

2.4. Elevation and soil data

Elevation data were obtained from Global 30 arcs Elevation (GTOPO30), with approximately 1-km horizontal resolution (USGS, 1996). In addition, ASTER Global Digital Elevation MODEL (ASTER GDEM) with 30-m horizontal resolution was used for calculating the terrain slope (Abrams et al., 2010). The spatial distributions of the annual irrigated corn and rain-fed harvested area (MIRCA2000) were obtained from Portmann et al. (2010) (Fig. S1), and were used to estimate the corn area ratio and to calculate the rain-fed and irrigated corn yield.

The cardinal inputs for each of three soil layer thicknesses (~15 cm, ~45 cm, and ~180 cm) were required by the EPIC model simulation. Soil texture, bulk density (including that of oven-dried soil), sand, silt, and clay content, pH, sum of bases (Ca, Mg, and K), organic carbon concentration, calcium carbonate content of soil, and cation exchange capacity were obtained from the Harmonized World Soil Database (HWSD, version 1.2; FAO, 2012) which is a 30 arcs raster database. Soil water content at wilting point and water content at field capacity were calculated based on HWSD using the Brooks–Corey equation (Brooks and Corey, 1966). Soil albedo was obtained from ECOCLIMAP, a global database of land surface parameters, at 1-km resolution (Champeaux et al., 2005; Masson et al., 2003).

2.5. Field management

The field management datasets required by the EPIC model were mainly planting and harvesting dates, irrigation operation date, amount, and times, and fertilizer application date, amount, and times. State-level planting and harvesting dates for corn were obtained from USDA (2010), based on the latest and the best information available (Fig. S2). The dates shown indicate planting and harvesting periods for most of the years based on 20 years of historical data estimates, as well as on the inherent knowledge of industry

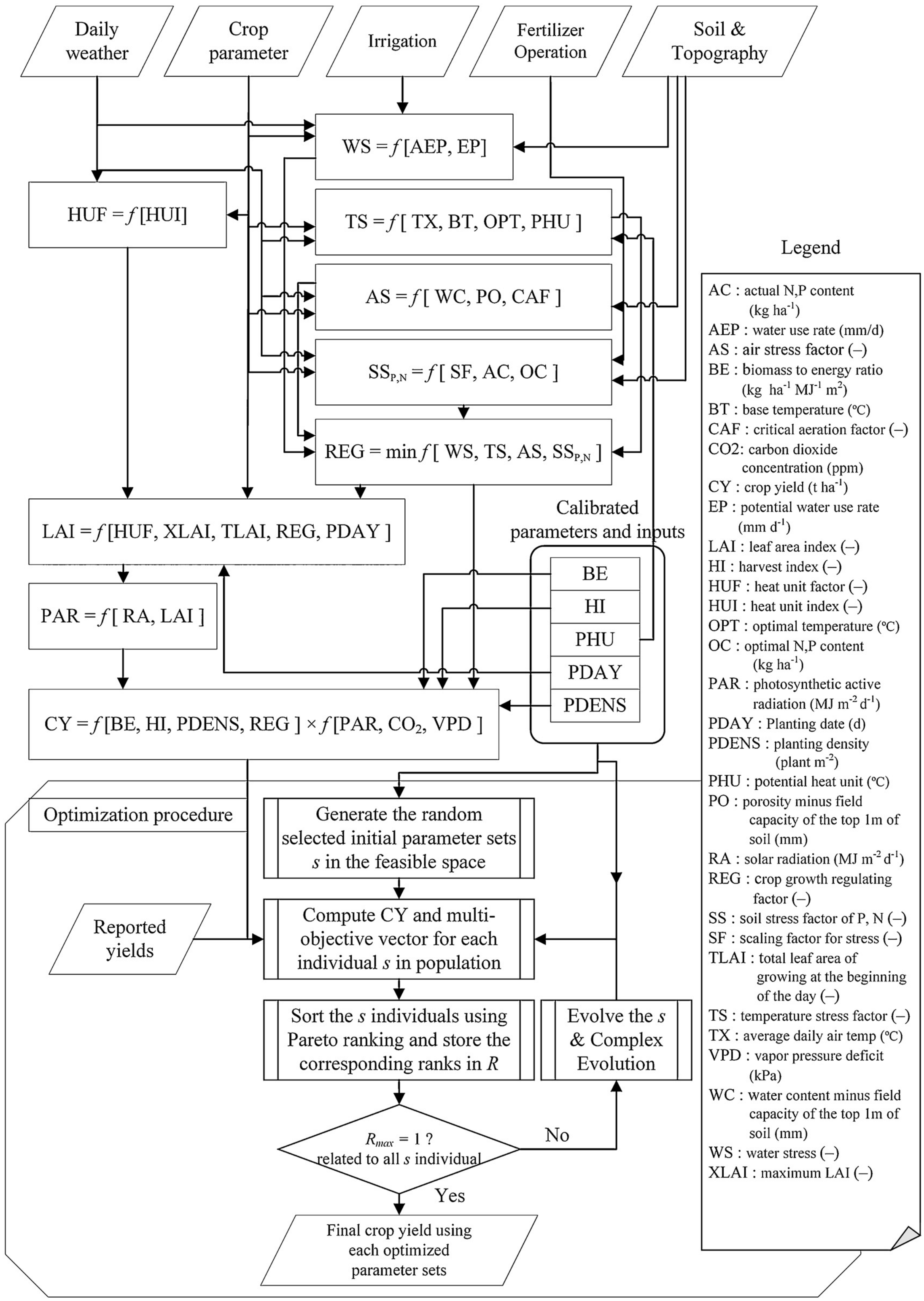

Fig. 1. Diagram of the crop yield simulation in the EPIC model and the flow chart of MOCOM-UA algorithm.

specialists. The present study used the periods when 15 to 85% of the crops were planted and harvested (the "most active" range of usual planting and harvesting dates) (USDA, 2010).

In the present study, rain-fed and irrigated regions were simulated separately using the annual harvested area of irrigated and rain-fed corn obtained from MIRCA2000. Irrigation occurred on the days when the ratio of dry biomass produced to potential corn production, given adequate water, fell below one. In other words, if the area equipped for irrigation is one, then there is no water stress. Irrigation water was applied between the minimum and maximum volume allowed for automatic irrigation in a single application, and these values were obtained from the default values of the model.

The nitrogen (N) and phosphorus (P) fertilizer application datasets were obtained from Global Fertilizer and Manure, Version 1 Data Collection (GFM) (Potter et al., 2010; SEDAC, 2015). In this study, the maximum annual fertilizers applied to the corn field

Table 2
EPIC initial parameters used for corn in this study (shaded rows are parameters and inputs used for auto calibration).

Parameter and inputs	Symbol[a]	Domain	Source
Biomass to energy ratio (kg ha^{-1} MJ^{-1} m^2)	BE	30–50	Personal setting based on Wang et al. (2005)
Harvest index	HI	0.45–0.60	Wang et al. (2005)
Potential heat units (°C)	PHU	1200–2400	Wang et al. (2005)
Planting dates (DOY)[b]	PDAY	Most active	USDA (2010)
Harvesting dates (DOY)[b]	HDAY	Most active	USDA (2010)
Planting density (plant m^{-2})	PDENS	5.6–9.0	Personal setting based on Widdicombe and Thelen (2002a, 2002b)
Optimal temperature (°C)	OPT	25	Kiniry et al. (1995)
Base temperature (°C)	BT	8	Kiniry et al. (1995)
Fraction of season when leaf area declines (–)	DLAI	0.7	Kiniry et al. (1995)
Potential leaf area index (–)	DMLA	6.5	Kiniry et al. (1995)
First point on optimal leaf area development curve (–)	DLAP1	15.05	Kiniry et al. (1995)
Second point on optimal leaf area development curve (–)	DLAP2	50.95	Kiniry et al. (1995)
Biomass-energy decline rate (–)	RBMD	1.0	Kiniry et al. (1995)
Leaf area index decline rate parameter (–)	RLAD	1.0	Kiniry et al. (1995)
Maximum rooting depth (m)	RDMX	2.0	Kiniry et al. (1995)

[a] Parameter symbols except for BE, PDAY, HDAY, PDENS, OPT, BT used in the EPIC model.
[b] See Fig. S2.

was calculated as the sum of applied N, P fertilizers and of applied N, P manure. Tillage operation was performed 30 days before and then 2 days before the planting date. N, P fertilizer was applied 30 days prior to planting in all years, and was also applied as the initial fertilizer during planting. Although the amount of applied N, P fertilizer for each grid cell during the growing period was determined by a simulated daily plant N, P stress factor obtained from default values, the total amount of N, P during the growing period never exceeded the values obtained from GFM. Other parameters and inputs related to crop, irrigation, tillage, and fertilizer were set to standard values contained in the EPIC datasets, except for the calibration parameters and inputs chosen for the uncertainty analysis.

2.6. Multi-objective optimization

2.6.1. The MOCOM-UA algorithm

The MOCOM-UA method is a global multi-objective optimization algorithm that is designed to be effective and efficient for a broad class of multi-objective problems. The MOCOM-UA strategy combines the strengths of the complex shuffling strategy with the competitive evolution and Pareto ranking, and the multi-objective downhill simplex evolution. This optimization algorithm has often been applied in hydrological models (e.g., Getirana, 2010; Leplastrier et al., 2002; Vrugt et al., 2003; Yapo et al., 1998), where its usefulness has been demonstrated, but there are only a few agricultural models that have used this algorithm. Basically, the optimization procedure with the MOCOM-UA consists of the following six discrete processes: (1) determination of the number of initial population size s (=120) to be randomly generated; (2) random distribution of initial samples of s points throughout the n (=5)-dimensional feasible parameter space; (3) evaluation of the functional multi-objective vector F for each individual s in a population; (4) ranking and sorting the population of s points using Pareto ranking procedure and storing the corresponding ranks ($R=\{r_i\}$, $i=1,\ldots,s$); the assigned ranks were 1,2,3,..., $R_{\max}$, where $R_{\max}=\max\{r_i\}\le s$ in a population of s individuals; (5) determining that the optimization process stops when all points $R_{\max}$ in the population have a rank equal to one; (6) evolving the sample population and applying the complex evolution to evolve the number of simplexes, which is equal to the number of points $N_{R\max}$ (the number having the largest rank). In the present study, the initial set of parameters and inputs of s points has been defined by a uniform random numbers in the feasible space. More detailed description on the multi-objective complex evolution, including multi-objective downhill simplex evolution (MOSIM) to evolve and improve $N_{R\max}$ points with the worst rank, can be found in Vrugt et al. (2003) and Yapo et al. (1998).

In the present study, the MOCOM-UA algorithm was implemented to the EPIC model. MOCOM-UA utilizes a rank-based selection procedure that enables the convergence of the selected points closest to the Pareto set. The final points by way of Pareto ranking, simplex generation, and simplex evolution were all mutually non-dominated and provided a fairly close approximation of the Pareto solution region. The flow chart of the MOCOM-UA algorithm is shown in Fig. 1.

2.6.2. Parameters and inputs selection

Although the use of more calibration parameters and inputs would contribute to the reduction of model uncertainty and would increase the number of the best attainable parameter and input values, it comes with a heavy computational cost. Therefore, efficient selection of calibration parameters and inputs is relatively important to enhance the reproducibility of corn yield with a light computational load. According to Williams et al. (2006) and Xiong et al. (2014), corn yield simulation presents a higher sensitivity when there is variation in the following three parameters: BE, HI, PHU, and two inputs: PDENS, PDAY. Therefore, these five parameters and inputs were considered in the process of automatic calibration to match the behavior of the real agricultural system. Here, BE is the dry biomass to energy ratio for converting intercepted solar radiation under non-stress conditions. HI is the ratio of harvested grain to total plant weight of a crop. PHU is the number of heat units, which was calculated by summing the mean daily temperatures and subtracting the base temperature during the growing season. The calibrated and other key parameters and inputs values in the present study are indicated in Table 2.

2.6.3. Objective functions

Automatic optimization procedures typically need the selection of an objective criterion that is efficient in searching the best parameter values of crop models to optimize a given objective function. For the hydrological model calibration, root mean square error and Nash-Sutcliffe criteria have been used frequently (e.g., Moriasi et al., 2012). However, knowledge on the beneficial objective function for a crop model is not necessarily enough. In the present study, the targeted parameters and inputs have been simultaneously calibrated using the four objective functions, to emphasize the minimization of errors of average, minimum and maximum yield over the simulation periods, and the inter-annual variation of yield against reported yield, in a multi-objective context using MOCOM-UA. The objective functions were defined as follows:

$$\mathrm{AVG} = \left| \left(\frac{S_{avg}}{O_{avg}} \right) - 1 \right| \quad (1)$$

$$R^2 = \left[\frac{\sum_{t=1}^{N} (O_t \times S_t) - \left(\sum_{t=1}^{N} O_t \times \sum_{t=1}^{N} S_t \right) / N}{\sqrt{\left[\left(\sum_{t=1}^{N} O_t^2 \right) - \left(\sum_{t=1}^{N} O_t \right)^2 / N \right] \times \left[\left(\sum_{t=1}^{N} S_t^2 \right) - \left(\sum_{t=1}^{N} S_t \right)^2 / N \right]}} \right] \quad (2)$$

$$\mathrm{MAX} = \left| \left(\frac{S_{max}}{O_{max}} \right) - 1 \right| \quad (3)$$

$$\mathrm{RRMSE} = \frac{1}{O_{avg}} \sqrt{\frac{1}{N} \sum_{t=1}^{N} (O_t - S_t)^2} \quad (4)$$

where S_{avg} and O_{avg} are the simulated and reported annual mean corn yield over the simulation periods, S_t and O_t are the yearly simulated and reported yield in the corresponding year t, and S_{max} and O_{max} are the maximum simulated and reported yield over the simulation periods, respectively, and the N was 12 for the study conducted that year. In this study, it was supposed that the AVG and MAX tend to emphasize minimization of errors of average and maximum corn yield over the simulation periods, respectively, while the R^2 (equals the square of the Pearson correlation coefficient (r)) and RRMSE provide a more consistent performance, which includes the temporal variability of yields, across the entire period. The multi-objective problem for the optimization process was defined as follows:

$$\underset{\theta}{\mathrm{minimize}} F(\theta) = \left(\mathrm{AVG}(\theta), \quad -1.0 \times R^2(\theta), \quad \mathrm{MAX}(\theta), \quad \mathrm{RRMSE}(\theta) \right) \quad (6)$$

where $F(\theta)$ is the multi-objective vector, θ is the optimized parameters.

3. Results

3.1. Spatial distribution of optimized parameters

Fig. 2 shows the progression and distribution of Pareto solutions resulting from the optimization process at two representative points in the Corn Belt. The initial population of randomly selected individuals in the objective space (in black), and final dots of non-dominated points (in red) are represented. After final iterations, (a total of 829,680 iterations for each of the 3457 grid cells) the black dots get closer to the optimal points (the origin in each Fig. 2; red dots). Although the Pareto front has the trade-off curve for the simple two-dimensional two-objective problem, the Pareto front for the complex four-objective problem indicated in Fig. 2 is not always clear compared to the two objective functions. However, it was verified that all the simplexes had been evolved exactly and the final points moved closer to the origin. Therefore, the non-dominated points selected from Pareto solution points (good solutions) for each of the 3457 grids were used as the model parameters and inputs to minimize each of the four individual criteria F, and the ensemble mean value across the simulation results (=120) obtained using the optimized parameters and inputs was calculated.

The optimized ensemble mean BE values (en-BE) obtained from non-dominated points at each grid cell increased compared to en-BE obtained from initial dominated points in most areas of the Corn Belt (Fig. 3a), while the en-BE values decreased in the central parts of North Dakota and South Dakota, the southern part of Texas, and the coastal region of the Eastern U.S. The optimized spatial-averaged en-BE values at state-level (state-BE) were especially larger in Iowa (5.3%), Illinois (2.8%), Nebraska (2.5%), Minnesota (7.5%), and Indiana (0.8%), which are the leading states of corn production, compared to the initial state-BE values. The state-BE values were identified as 39.5 kg ha^{-1} MJ^{-1} m^2 in Iowa, 38.5 kg ha^{-1} MJ^{-1} m^2 in Illinois, 38.4 kg ha^{-1} MJ^{-1} m^2 in Nebraska, and 40.4 kg ha^{-1} MJ^{-1} m^2 in Minnesota, and 37.8 kg ha^{-1} MJ^{-1} m^2 in Indiana through the automatic optimization search (Table 3).

Correlation coefficients (r) between the optimized en-BE per county-level and county-level annual mean reported yield over the period 1999–2010 were 0.39 (n = 256) for Iowa, 0.38 (n = 239) for Illinois, 0.21 (n = 305) for Nebraska, 0.34 (n = 214) for Minnesota, and 0.25 (n = 152) for Indiana. For these states, the r values were statistically significant ($p < 0.05$, two-tailed probability) (Table 4). The r values were also statistically significant for North Dakota, South Dakota, Ohio, Pennsylvania, Maryland, South Carolina, Texas, and Mississippi ($p < 0.05$, two-tailed probability). Adjusted state-BE was close to the 35.3 to 40.4 kg ha^{-1} MJ^{-1} m^2 range for all the states (Table 3). These values were lower compared to the previous modeling values of 47.0 kg ha^{-1} MJ^{-1} m^2, 43.3 kg ha^{-1} MJ^{-1} m^2, obtained from the studies of Bulatewicz et al. (2009) and Yang et al. (2004), respectively. However, they were consistent with 39.8 kg ha^{-1} MJ^{-1} m^2, and 35.0 to 40.0 kg ha^{-1} MJ^{-1} m^2, the values obtained from the studies of Kiniry et al. (2004) and Stöckle et al. (2003), even though these studies used different calculation methods and environmental conditions.

Fig. 3b shows the spatial pattern of percentage change in ensemble mean value of HI, between initial and final sets. Adjusted state-level HI increased compared to the HI obtained from using the initial sets in major corn growing states such as Minnesota (1.7%), Iowa (1.5%), and Illinois (0.9%), while it decreased in the southern and coastal eastern parts of the U.S. (Fig. 3b). The r between the optimized ensemble mean HI value per county-level and county-level annual mean reported yield over the period 1999–2010 was statistically significant ($p < 0.05$, two-tailed probability) in North Dakota, South Dakota, Nebraska, Minnesota, Iowa, Missouri, Wisconsin, Illinois, North Carolina, and Texas. Moreover, a relatively larger adjusted state-level HI value (=0.53) occurred in the major corn area, such as Minnesota, Iowa, Illinois, and lower HI values were seen in the southern and the eastern parts of the U.S. (Table 3). The spatial variability of the ensemble mean values of HI, PDENS and PDAY was relatively smaller than that of BE values (Table 3). In other words, HI, PDENS, and PDAY need not necessarily be meticulously determined across the heterogeneous units.

The optimized ensemble mean PHU values obtained using the final sets increased more than 8% on an average in the major corn growing regions compared to the ensemble mean PHU values obtained using the initial sets (Fig. 3c). The largest adjusted state-level PHU (>1900 °C) occurred in Nebraska, Iowa, Illinois, Indiana, Arkansas, Louisiana, and Mississippi and the lowest (<1600 °C) was found in North and South Carolina (Table 3). The r between the ensemble mean PHU values per county-level and county-level annual mean reported yield over the period 1999–2010 was significant ($p < 0.05$, two-tailed probability) in South Dakota, Nebraska, Iowa, Wisconsin, Illinois, Kentucky, Tennessee, Pennsylvania, South Carolina, and Texas. On the other hand, the r between the ensemble mean PDENS, PDAY values per county-level and county-level annual mean reported yield over the period 1999–2010 was not significant ($p > 0.05$) for all states except for PDAY in Texas. As a result of the different trends of calibration parameter evolution, the adjusted BE, HI and PHU would have relatively stronger effects on the reported yield, and these would be relatively more effective parameters in improving the spatial agreement and temporal variability of yield.

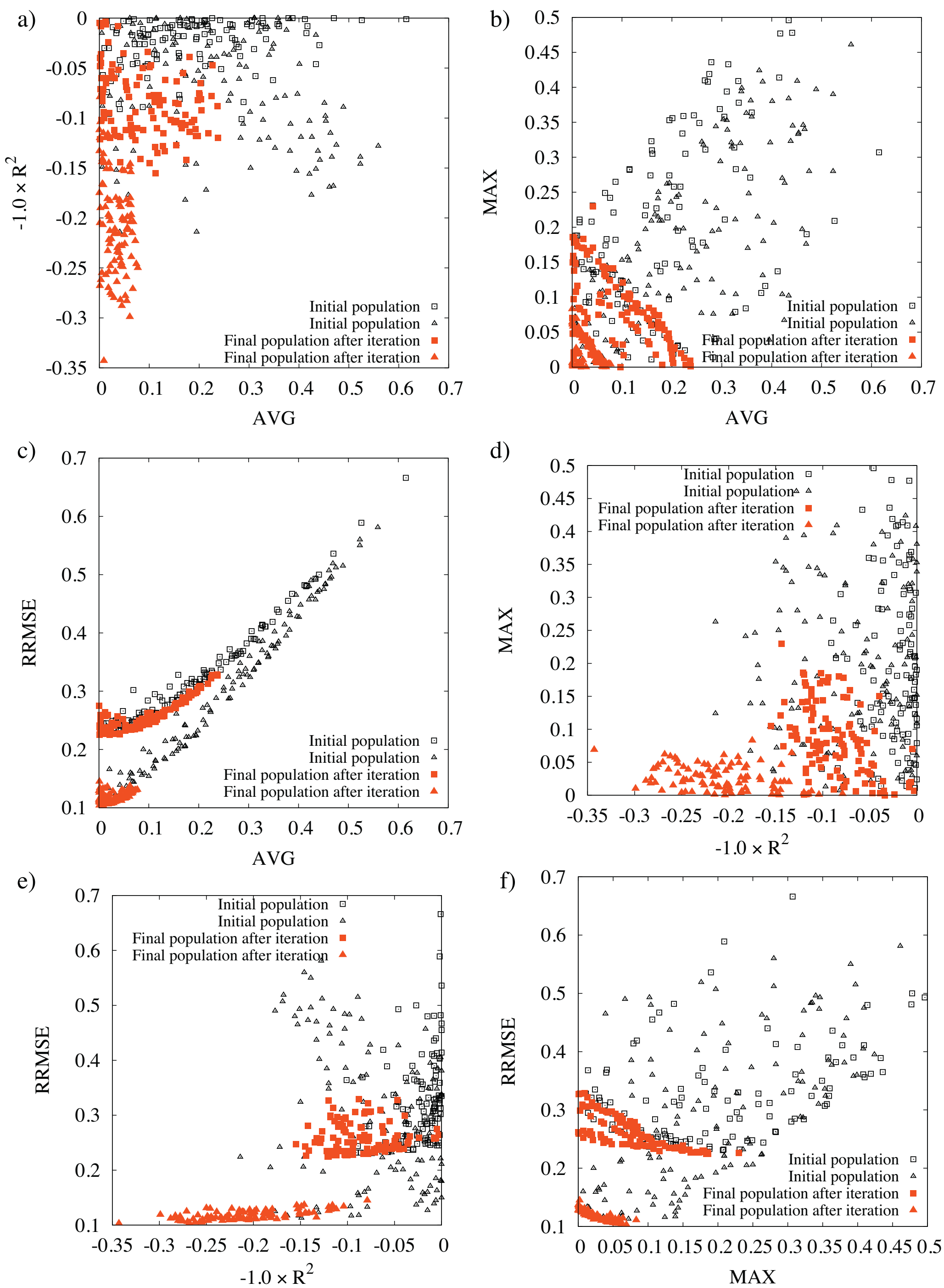

Fig. 2. Pareto solutions from the optimization process for a four-objective (AVG, R^2, MAX, RRMSE) problem at two representative corn grid points (square: 42.125°N, 98.125°W, triangle: 41.125°N, 96.125°W, initial populations (in black), final populations (in red)). ((a) AVG vs $-1.0 \times R^2$, (b) AVG vs MAX, (c) AVG vs RRMSE, (d) $-1.0 \times R^2$ vs MAX, (e) $-1.0 \times R^2$ vs RRMSE, (f) MAX vs RRMSE). For more explanation, see text. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3.2. *Reproducibility of corn yield*

Fig. 4a and b shows the simulated ensemble mean yield and the reported yield, respectively, over the period 1999–2010. The spatial pattern of simulated yield was generally consistent with the pattern of reported yield in the main corn production states, i.e., Nebraska, Minnesota, Iowa, Illinois, and Indiana, which account for more than 60% of the total national production (USDA, 2014b). However, the simulated yield was underestimated in the higher reported yield areas in other parts of the Corn Belt and in the southern part of the U.S., and was overestimated in the relatively lower reported yield areas (around the Corn Belt) and in the coastal region of the Eastern U.S. The difference in simulated and reported yield was relatively large in the southern region of the U.S. (Fig. 4c). Spatial R^2 between the ensemble mean and the reported yield had 0.10 as the 10th percentile, 0.31 as the average, and 0.56 as the 90th percentile value.

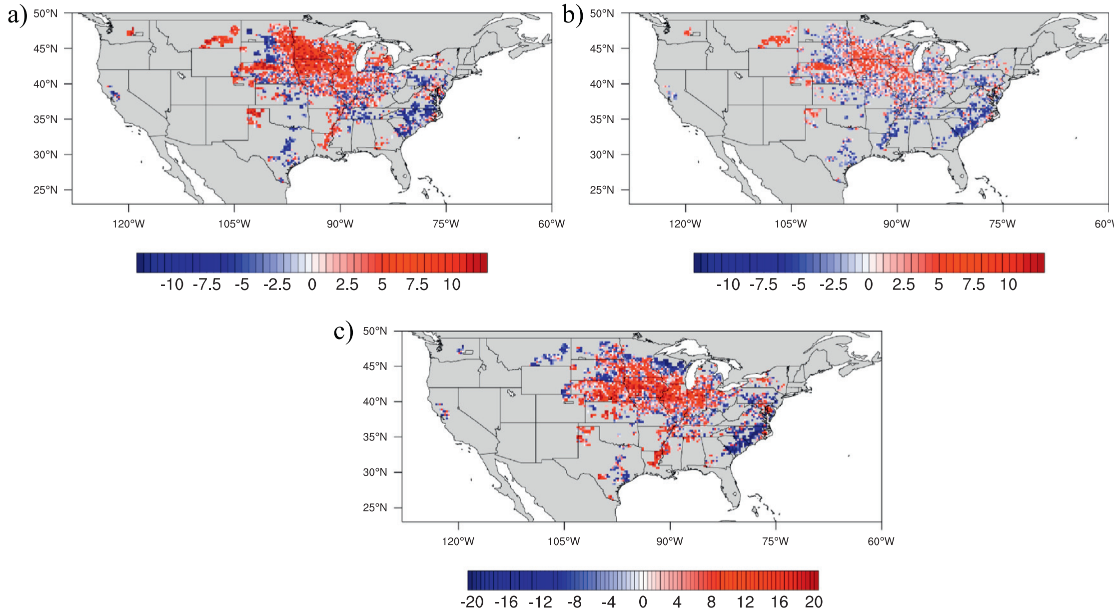

Fig. 3. The spatial patterns of ensemble mean values of the percentage changes. Percentage changes represent differences between values obtained using initial and final parameter sets for (a) BE, (b) HI, and (c) PHU.

Spatial RRMSE had 13% as the 10th percentile, 23% as the average, and 37% as the 90th percentile value. In addition, spatial absolute values of ensemble mean value of the difference between peak simulated and reported yield over the period 1999–2010 (ABSPEAK) had 0.37 t ha^{-1} as the 10th percentile, 0.92 t ha^{-1} as the average, and 1.62 t ha^{-1} as the 90th percentile value. Paired *t*-test showed that the difference in yield between the ensemble mean values of simulated and reported yield for the period 1999–2010 was statistically significant in 527 grid cells out of 3457 grid cells ($p < 0.05$; two-tailed probability).

The reproducibility related to the spatial agreement and temporal variability of yield tended to be inferior with a lower R^2 and a higher RRMSE, ABSPEAK in the minor corn area, and tended to be superior with a higher R^2 and lower RRMSE, ABSPEAK in the major corn area (Figs. 4 and 5). Even after the use of converged optimal model parameter and input sets obtained using MOCOM-UA optimization, the simulation results showed a certain spatial width to yield reproducibility, and errors between simulated and reported yield were observed. This output uncertainty was attributed to the uncertainties in model parameters and inputs values.

3.3. Effect of the parameter optimization on reproducibility of yield

The output uncertainty may be reduced using the optimized model parameters through auto calibration. In particular, BE, HI

Table 3
Estimated spatial-averaged ensemble mean values and standard deviations at state-level.

State	BE		HI		PDENS		PDAY		PHU	
	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
North Dakota	37.9	2.4	0.52	0.015	7.91	0.13	136.	2.5	1768	142
South Dakota	37.2	2.4	0.51	0.016	7.89	0.13	136.	2.6	1797	172
Nebraska	38.4	2.2	0.52	0.020	7.90	0.13	127.	1.8	1913	146
Minnesota	40.4	1.3	0.53	0.017	7.91	0.12	128.	2.4	1861	157
Iowa	39.5	1.7	0.53	0.017	7.91	0.14	127.	2.4	1979	152
Missouri	37.9	1.6	0.52	0.015	7.91	0.12	125.	5.0	1809	139
Wisconsin	39.3	1.4	0.52	0.016	7.91	0.13	134.	2.7	1726	193
Illinois	38.5	1.8	0.53	0.016	7.91	0.14	128.	3.6	1925	145
Michigan	38.0	1.8	0.52	0.015	7.88	0.13	135.	2.4	1798	148
Indiana	37.8	1.8	0.52	0.014	7.87	0.13	137.	3.4	1944	135
Kentucky	37.8	1.9	0.51	0.015	7.88	0.15	125.	3.8	1795	143
Tennessee	36.1	1.9	0.51	0.017	7.91	0.14	116.	3.7	1798	170
Ohio	37.5	1.4	0.52	0.014	7.87	0.12	130.	2.6	1814	140
New York	38.1	1.7	0.52	0.014	7.90	0.13	147.	4.5	1818	155
Pennsylvania	36.0	1.5	0.51	0.014	7.88	0.11	138.	1.4	1714	169
Maryland	38.0	2.2	0.52	0.016	7.88	0.15	131.	2.6	1867	188
Virginia	36.6	1.8	0.51	0.017	7.88	0.13	124.	4.2	1723	152
North Carolina	35.3	2.1	0.50	0.019	7.89	0.13	108.	1.4	1590	223
South Carolina	35.7	1.9	0.49	0.014	7.85	0.13	95.8	3.2	1515	173
Texas	37.3	2.6	0.52	0.019	7.91	0.15	101.7	7.6	1815	194
Arkansas	38.8	1.5	0.51	0.017	7.89	0.13	104.7	2.0	1959	125
Louisiana	39.3	1.4	0.50	0.017	7.94	0.14	89.08	2.0	2059	94
Mississippi	38.2	1.7	0.50	0.015	7.90	0.13	102.8	3.2	1919	173

Table 4
Correlation coefficients between optimized ensemble mean values per county-level and county-level annual mean reported yield over the period 1999–2010. Shaded parts in the table indicate statistically significant values ($p < 0.05$).

State	BE	HI	PDENS	PDAY	PHU
North Dakota	0.69	0.36	0.10	0.10	0.06
South Dakota	0.69	0.25	0.05	0.06	0.30
Nebraska	0.21	0.34	0.00	0.01	0.31
Minnesota	0.34	0.47	0.00	0.02	0.02
Iowa	0.39	0.19	0.00	0.00	0.18
Missouri	0.00	0.33	0.01	0.00	0.02
Wisconsin	0.06	0.25	0.02	0.03	0.33
Illinois	0.38	0.30	0.01	0.00	0.41
Michigan	0.04	0.00	0.03	0.08	0.05
Indiana	0.25	0.07	0.00	0.05	0.08
Kentucky	0.01	0.07	0.01	0.00	0.23
Tennessee	0.04	0.04	0.01	0.00	0.35
Ohio	0.18	0.13	0.00	0.00	0.15
New York	0.04	0.04	0.00	0.01	0.01
Pennsylvania	0.35	0.05	0.00	0.02	0.40
Maryland	0.18	0.02	0.00	0.03	0.08
Virginia	0.07	0.16	0.02	0.18	0.00
North Carolina	0.08	0.23	0.02	0.05	0.16
South Carolina	0.69	0.04	0.09	0.15	0.46
Texas	0.78	0.51	0.12	0.32	0.35
Arkansas	0.03	0.16	0.21	0.00	0.01
Louisiana	0.01	0.17	0.05	0.02	0.05
Mississippi	0.57	0.18	0.01	0.00	0.39

and PHU values would have especially large impact on the performance of simulation results (Section 3.1). Therefore, in order to investigate the improvement effect of the corn yield reproducibility by using MOCOM-UA, the ensemble mean values of R^2, RRMSE, and ABSPEAK obtained using both initial and final sets were calculated.

Fig. 6 shows the distribution of the reported and simulated yield using both initial and final sets for the periods 1999–2010. In Fig. 6, the upper and lower hinges of the boxes indicate the 10th and 90th percentile, respectively, in the ensemble values resulting from the different calibrated parameters. Even though a specific bias between simulated and reported yield for the period 1999–2010 can be seen, a reduction in the width of the uncertainty band is also clearly observed by using the optimized parameters and inputs.

4. Discussion

4.1. Reproducibility under extreme weather event

The use of the optimized parameters should be effective in improving the spatial agreement, the inter-annual variability and in reducing the width of the uncertainty band. For example, the drought in 2002 affected the whole area of the U.S. Corn Belt, with yields decreasing by more than 10% of the normal corn yield. The regions ranging from Illinois to the east coast were faced with the most serious damage in 2002 (Sakamoto et al., 2014). In this study, the spatial-averaged reported yield (7.9 t ha^{-1}) in Illinois for 2002 was within the width of the uncertainty band (from 6.8 t ha^{-1} to 10.7 t ha^{-1}) obtained using the adjusted parameters (Fig. 6h), but the ensemble mean yield (8.9 t ha^{-1}) was overestimated by

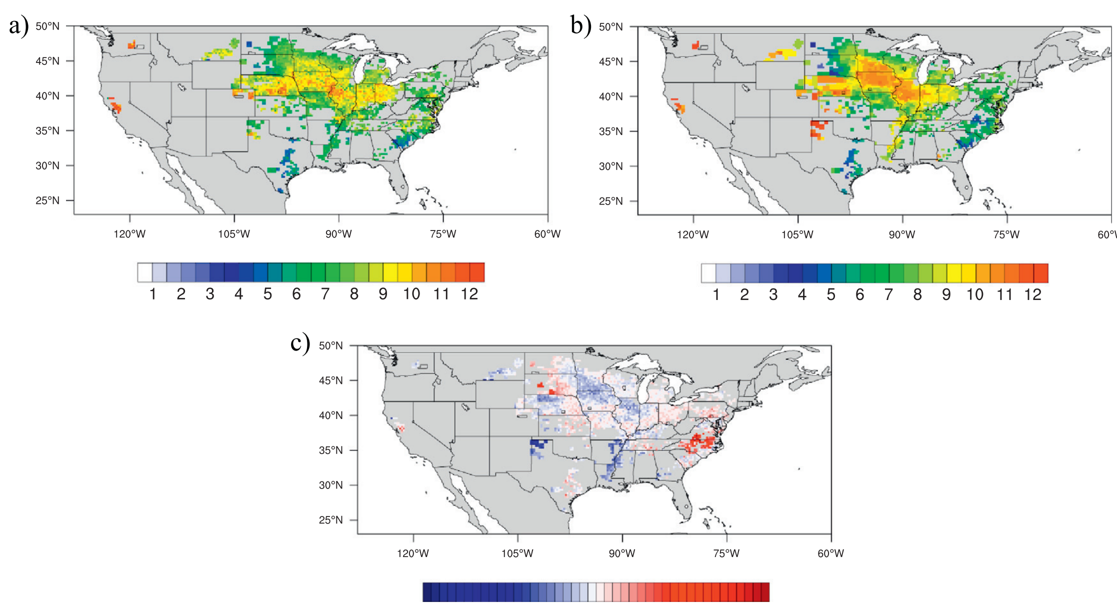

Fig. 4. Spatial patterns of average corn yield for the period 1999–2010. (a) Ensemble mean yield, (b) reported yield, and (c) ((a)–(b)/(b)).

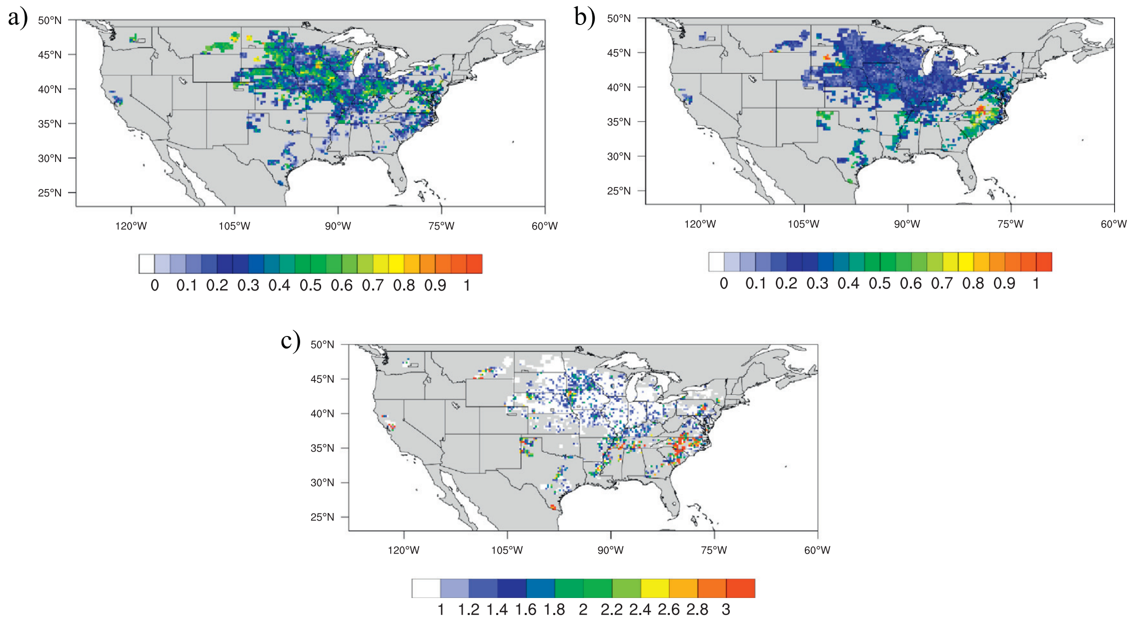

Fig. 5. Spatial patterns of ensemble mean value of (a) R^2, (b) RRMSE, and (c) ABSPEAK (absolute values of ensemble mean value of the difference between peak simulated and reported yield) between simulated and reported yield for the period 1999–2010.

1.0 t ha^{-1}. The bias in yield between simulated and reported is not limited to 2002. The reported yield in Indiana for 2002 (7.1 t ha^{-1}) was more than 20% lower than the annual average yield for the period 1999–2010. In this study, although the ensemble mean yield for 2002 was lower than the other years, it was overestimated by 1.2 t ha^{-1} compared to the reported yield (Fig. 6j). Likewise, the ensemble mean yield in Ohio and Pennsylvania for 2002 (8.4 t ha^{-1} and 7.4 t ha^{-1}) was overestimated by 3.0 t ha^{-1} and 3.1 t ha^{-1} compared to the reported yield, respectively (Fig. 6m and o). In addition, the width of the uncertainty band using the different combinations of final sets decreased compared to that using initial sets, but the difference in simulated and reported mean yield for 2002 increased.

These results indicate that it is difficult to represent rapid yield declines caused by natural disasters, pests, and diseases that occur during the crop-growing period, but the width of the uncertainty band obtained in this study using the final sets included the reported yields for many states and years (Fig. 6). However, in order to reduce the width of the uncertainty band further while increasing model reliability, further investigations using more soil, climate-related, and water-sensitive optimization parameters are needed. These should help to clearly identify the quantitative effects of the calibration parameters and inputs on the inter-annual variation of yield in addition to improving the reproducibility under extreme weather events.

4.2. Uncertainties

Crop simulation under current climate conditions is needed to test the uncertainties of the model and to increase the reliability of assessments for future climate change impacts. Generally, the accuracy and reliability of simulation results obtained from crop models depend on the precision and reliability of model parameters and inputs. In this study, the difference between spatial- and period-averaged ensemble mean yield and reported yield was within ±1.0 t ha^{-1} in the major corn area (e.g., Nebraska: −0.5 t ha^{-1}, Minnesota 1.0 t ha^{-1}, Iowa: −0.7 t ha^{-1}, Illinois: −0.6 t ha^{-1}, Indiana: −0.2 t ha^{-1}, and Ohio: 0.4 t ha^{-1}). On the other hand, crop simulation results in the minor corn area, like the southern and eastern parts of the U.S., had relatively large errors (Figs. 4–6). The main causes for errors between the simulated and reported yield are as follows: (1) uncertainty of fertilizer and manure application rates; (2) uncertainty of soil information; (3) reliability of the corn growing area; (4) uncertainties concerning the model input datasets; (5) reliability of reported datasets; and (6) uncertainties related to pest, diseases, and extreme weather events, etc.

The model parameters and inputs related to fertilizer and manure application have a large effect on crop growth (Stehfest et al., 2007). The N, P fertilizer dataset was computed by fusing global maps of harvested areas for 175 crops with national information on fertilizer use for each crop. The N, P values in manure production were derived based on the N, P content of the manure produced by the total number of livestock located within each grid cell. The value of these datasets is averaged for the period 1994–2001 (SEDAC, 2015). Moreover, Stehfest et al. (2007) indicated that the large discrepancies between nitrogen application rates and the amount of nitrogen removed cause a significant error in crop yields. As mentioned previously, relatively large errors between the simulated and reported yield were found in the southern and coastal regions of the Eastern U.S. This result may indicate that heterogeneous land use within the grid area promotes uncertainty to crop simulation (van Ittersum et al., 2013). The more reliable input datasets related to fertility, drainage, and depth traits of soils in those regions is necessary for accurate EPIC model simulation.

Irrigation is key for higher agricultural production and stable crop quality and the data on the irrigated area contribute toward estimating the state and nation-level average corn yield. In this study, it is assumed that automatic irrigation was performed when soil moisture in the root zone was less than a specified value below the field capacity. It should also be mentioned that the assumptions of irrigation trigger that were made in this study (described in Section 2.5) may not correspond exactly with what occurred in the actual site in reality. For example, the ensemble mean yield obtained for the Mississippi river basin was underestimated compared to the reported yield (Fig. 4c), which might have been due to the inability to predict higher water stress days that could have led to forced irrigation at that time. It is not easy to accurately and quantitatively estimate uncertainties relating to plant stress, such as those caused by unexpected water and nutrient scarcity.

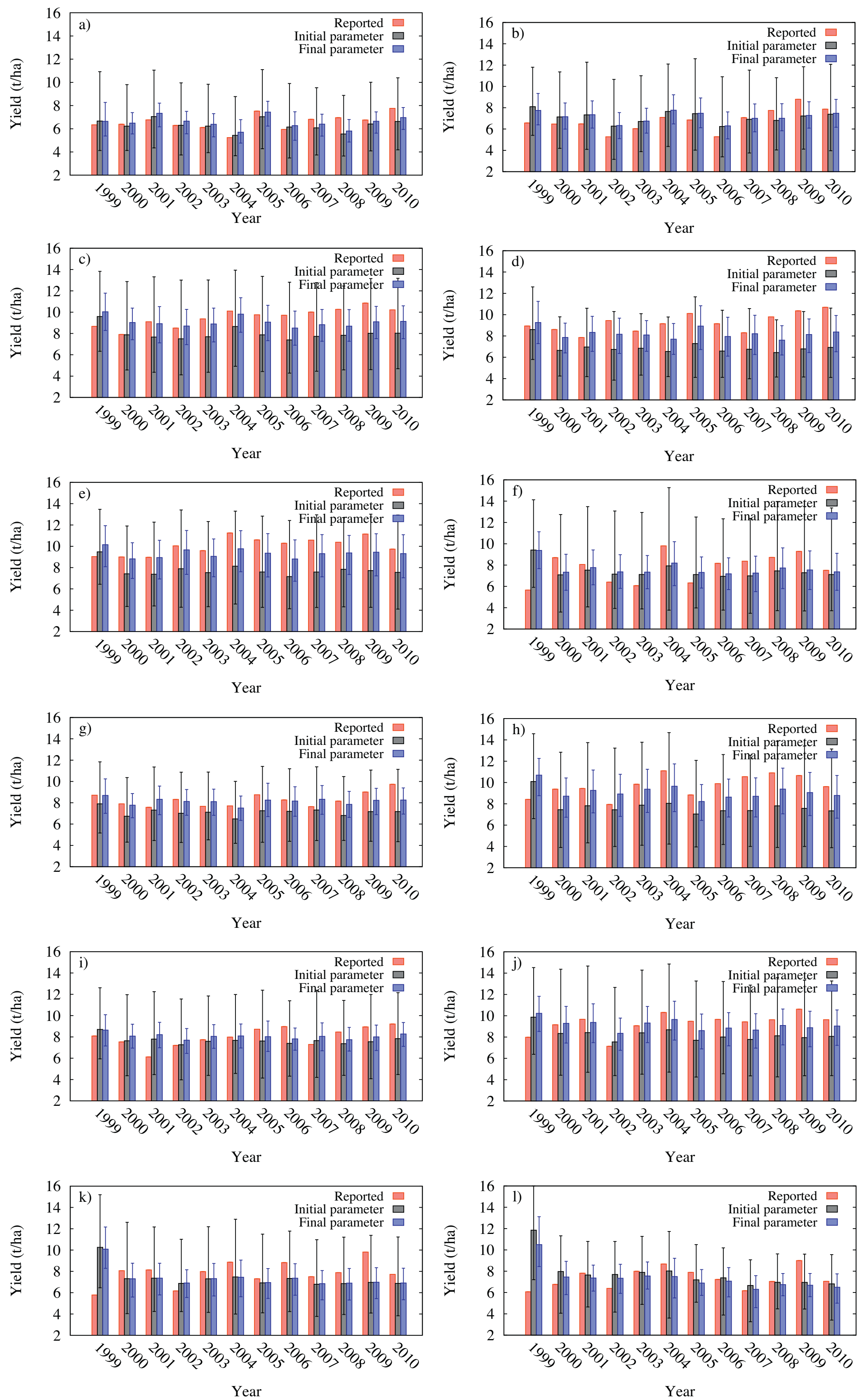

Fig. 6. Reported yield and the ensemble mean yield for each state obtained using initial and final parameter sets for the period 1999–2010. Vertical bars indicate 10th percentile and 90th percentile yield of ensemble simulated yield values. (a) North Dakota, (b) South Dakota, (c) Nebraska, (d) Minnesota, (e) Iowa, (f) Missouri, (g) Wisconsin, (h) Illinois, (i) Michigan, (j) Indiana, (k) Kentucky, (l) Tennessee, (m) Ohio, (n) New York, (o) Pennsylvania, (p) Maryland, (q) Virginia, (r) North Carolina, (s) South Carolina, (t) Texas, (u) Arkansas, (v) Louisiana, (w) Mississippi).

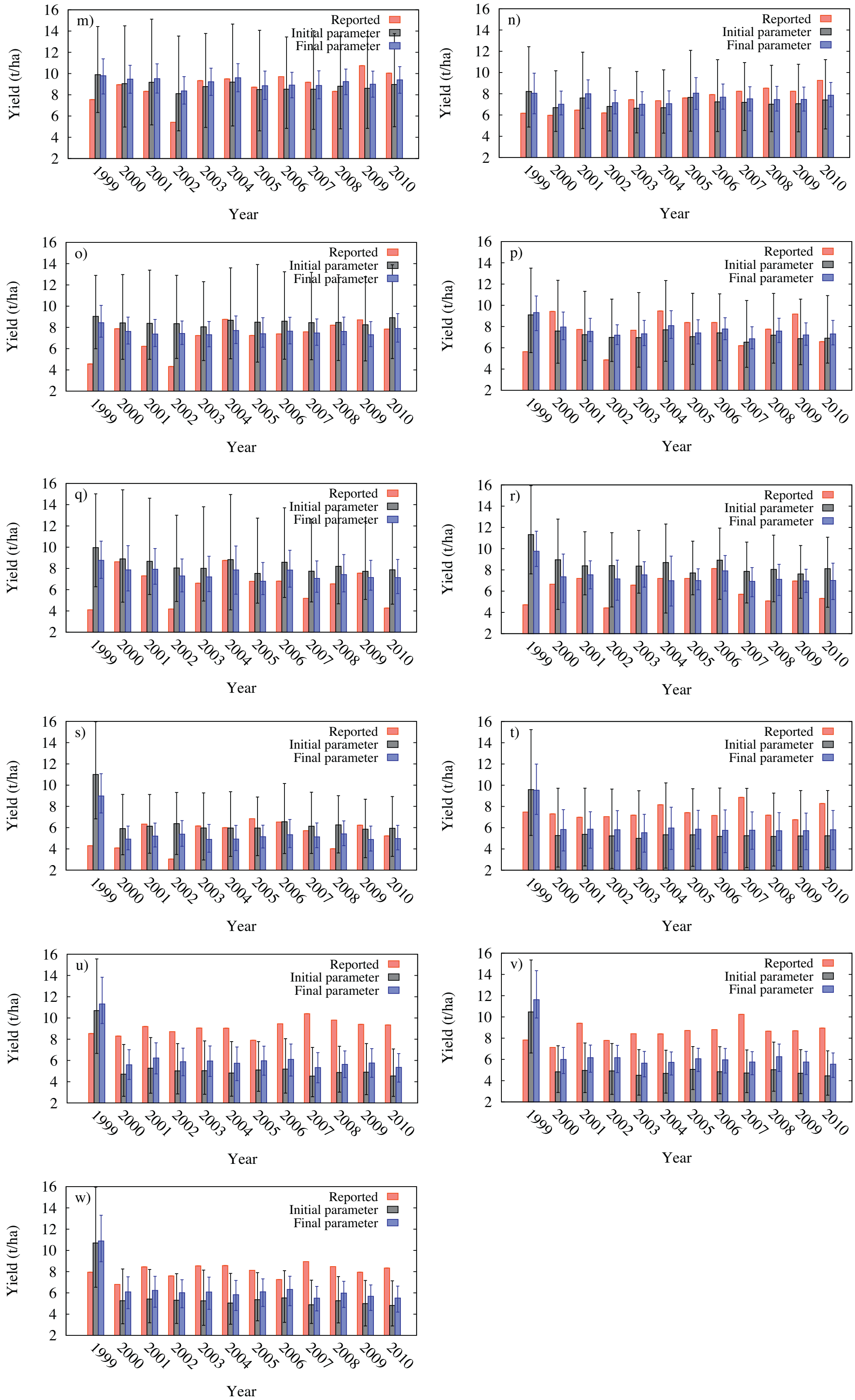

Fig. 6. (*Continued*).

Other uncertainty factors that might influence the model predictions are assumptions made on the frequency of corn cultivation, soil profile and crop distribution. In the U.S. corn and soybean crop rotation is generally performed in the Corn Belt (Sakamoto et al., 2014) and so the same crop species is not grown on the same grid every year. NASS, an agency of the USDA, uses farmer surveys and several other methods to calculate census estimates of farmland acreage across the country. However, not every farmer returns a census form and the response rate has been trending downward. In addition, the Census of Agriculture and other NASS publications offer the most comprehensive, detailed information about American farming available, but it should not be forgotten that these figures are just estimates gleaned from an enormous and tangled set of raw data—not ironclad, indisputable truths (Modern farmer, 2014). Therefore, the assumption made in our model that corn cultivation was conducted at all grid cells in the county every year may not represent the real situation. Moreover, accurate datasets related to soil within the gridded data are indispensable for accurately simulating yields, but soil profile data in the present study may not precisely reflect the actual variability in the soil types of the U.S. corn area. The uncertainty of heterogeneous crop distribution could be reduced by using higher spatial resolution and reliable input datasets. The results obtained must also be evaluated using a more reliable reported yield.

The poor reproducibility of inter-annual variability in this study is consistent with what was obtained from past research (Xiong et al., 2014). This can be attributed to a range of factors, but probably the most important factor would be the homogeneity of the model parameters and inputs (except for the calibrated parameters and inputs related to crop growth) and the uncertainty of crop management inputs. In reality, the field operation schedule and the management method depend on the individual farmers, and their management in turn will depend on several factors, such as the weather condition, food supply and demand, market, and traditional culture. In addition, mechanization of the agricultural machinery for corn farming and labor-saving operations would also contribute to the uncertainty factors influencing the results. In addition, because of use of single cultivar, single managements, it is difficult to predict the true aggregated corn yield.

4.3. Issues and meaning of the study

Given all these counteracting factors and issues involved, why is this study important and how does it contribute toward better and more sustainable agriculture? Within the limitations of the number of reliable model parameters and computational resources, this research has suggested a few possibilities to perform a more accurate crop yield simulation with reduced model uncertainty. First, it identified a useful and practical modeling approach to determine the optimal BE, HI, and PHU. Crop growth modeling is likely to have little impact when the parameter setting is not correctly done. Therefore, an automatic calibration using multi-objective global optimization for crop models is a very important process to find the set of all non-dominated solutions. In the past research, model parameters relating to agricultural production process and farm management have been obtained from experiments at the field scale, which measured detailed weather conditions, plant growth, and soil data etc. At relatively large scales, however, region-specific phenology parameters have only been obtained from past literature or research owing to the difficulties in obtaining and applying reliable information and details on a regional basis (Balkovič et al., 2013; Brown et al., 2000; Easterling et al., 1998; Izaurralde et al., 2003; Ko et al., 2009).

Next, this model provides a better way to optimize parameters and to reduce uncertainty bands in the model. Even though crop model parameterization constitutes an indispensable process in accurate crop simulation, parameter determination is nearly a "black box", with precious little information and details available from past research, making it extremely difficult for users to obtain a holistic understanding of the methods. The projected multi-objective optimization of crop model parameters contributes toward (1) mitigating the width of the uncertainty band and reducing the spatio-temporal errors between the simulated and reported yield, and (2) executing the sensitivity and uncertainty analysis of yield using the crop model for given local and large-scale field conditions. Even though calibrations using a lot more crop model parameters, such as optimum temperature, maximum leaf area index, and water and soil stress factors, would be effective for bias reduction and would bring better spatial agreement and inter-annual variability, they would require an expensive computer with more speed and power. A large initial population size may produce more beneficial Pareto solution sets but would also increase the number of iterations required for convergence of the solution. Further, to particularly enhance the model utility in low data regions, the quantitative and qualitative effect of the number, the type and the importance of calibration parameter and the objective function on yield reproducibility should be investigated further.

5. Conclusions

The objective of the present study was to investigate the effectiveness and efficiency of the MOCOM-UA algorithm for corn yield simulation with the EPIC model. The large-scale crop model simulation presents a wide range of uncertainties for the corn yield. The model represents crop growth processes and addresses some of the uncertainties, but a more reliable crop simulation is required to investigate the effect of climatic variability and soil environment on crop yield, and to characterize and quantify climate change impacts on agriculture. The results suggested that simulated corn yield is highly sensitive to the model parameters BE, HA, and PHU. Multi-objective optimization using the MOCOM-UA algorithm contributed to the reduction of the width of the uncertainty band and improvement of spatial pattern and temporal variability of corn yield. The ensemble mean yield obtained using the algorithm agreed well with the reported yield level (spatial-averaged RRMSE = 23% across all cultivated grid), and the EPIC model displayed better performance in the major corn area that had relatively accurate input datasets with low uncertainty (e.g., crop parameter, cultivated area, field management, and reported yield). However, the measurement errors (R^2, RRMSE, and ABSPEAK) between the simulated and reported yield were relatively larger in the minor corn area with lower yield and corn area ratio.

To summarize, the multi-objective automatic calibration procedure proposed in this study is a good tool for the identification of critical model parameters and for understanding model uncertainties, as well as for improving spatial agreement and temporal variability of corn yield. Future objectives of the study are: (1) reducing the width of the uncertainty band and improving the reproducibility of yield; (2) improving model calibration by increasing or selecting better calibration parameters and objective functions, which will be needed to address spatial agreement and temporal variability of crop yield more accurately.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecolmodel.2015.11.006.

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