

Analysis of parameter uncertainty in model simulations of irrigated and rainfed agroecosystems

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ABSTRACT

Crop water production functions (quantifying crop yield as a function of irrigation rate) can help in the design of management systems that reduce the water footprint. We examined the role of parameter uncertainties in characterizing production functions using the DayCent agroecosystem model. A global sensitivity analysis was conducted to identify the model parameters associated with the greatest uncertainties in model responses. Under both irrigated and non-irrigated conditions, growth/production-related parameters had relatively more impact on grain yield than did soil-related parameters. Under non-irrigated conditions, there was greater sensitivity to evapotranspiration related parameters. We then used the DREAM method, a Markov Chain-Monte Carlo (MCMC) Bayesian approach, to determine the posterior distributions of the selected parameters. The DREAM method produced good estimates for the posterior distribution of the critical parameters. The utility of water production functions as predictive tools to guide water management decisions is greatly enhanced by incorporating rigorous estimates of uncertainty.

Software availability

Program title: DayCent model

Developer: W. J. Parton, S. J. Del Grosso, S. Ogle, K. Paustian, Y. Zhang

Contact address: Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, CO, USA Telephone (970) 491–2195
Email address Yao.Zhang@colostate.edu

Year first available: 1998

Hardware required: PC

Software required: Windows or Linux

Availability and cost: Available on request; Free

Program title: DREAM (DiffeRential Evolution Adaptive Metropolis) package for R

Developer: J.A. Vrugt, C.J.F. Ter Braak et al

Contact address: Department of Civil and Environmental Engineering, The University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249, USA. Email address john.joseph@utsa.edu (J.F. Joseph)

Availability and cost: <http://dream.r-forge.r-project.org/>; Free

1. Introduction

In the irrigated river basins of arid and semi-arid regions in the western United States, vulnerability to water shortage poses a significant risk to agricultural production (Ahuja et al., 2008; Doorenbos and Kasam, 1979; Dozier et al., 2017). Large amounts of water from surface and underground sources are applied as irrigation to maintain high crop yields. Irrigation withdrawals in the US account for approximately 38% of total freshwater withdrawals (Maupin et al., 2014). The increasing demand for water from municipal users due to rapid population growth and urbanization as well as demands for other industrial and environmental uses increasingly limit the availability of water for agriculture (Colorado Water Conservation Board, 2010; Vorosmarty et al., 2000). Extended drought periods in a changing climate and declining groundwater levels are expected to further exacerbate the situation (Colorado Water Conservation Board, 2010; McGuire, 2014). Understanding the response of cropping systems to changes in irrigation levels is essential for reducing the water footprint of agricultural crops while maintaining production levels (Feres and Soriano, 2007; Saseendran et al., 2014; Trout et al., 2010). The estimations of the responses can be used in complex economic and social analyses for decision support; the optimal

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irrigation amounts are often determined by various economic and social factors (Dozier et al., 2017).

Dynamic crop models are valuable tools for the estimation of the crop yield response to water (Brumbelow and Georgakakos, 2007; Garcia-Vila and Fereres, 2012; Saseendran et al., 2014). However, simulation models are only approximate representations of real world systems and thus bear uncertainties in simulating system behavior. The predictions of dynamic crop models are influenced by inputs (meteorological, soil, and land use), uncertain model parameters, the limitation of the mathematical representation of real world processes, and uncertainty in the observed data that are used for calibration purposes. All of these components need to be considered in assessing the uncertainty in crop model predictions (Confalonieri et al., 2016).

Sources of modeling uncertainties can be grouped into three categories: input, structural, and parameter uncertainties (Haefner, 2005). Input uncertainty is from errors in input forcing (e.g. precipitation or soil texture of a field). Model structures are invariably incomplete and uncertain due to the simplification of real world processes, lack of knowledge about some processes, and from neglecting to include some processes that are deemed insignificant for pragmatic considerations. Finally, model parameters, time-invariant coefficients that are treated as constants and are estimated by means of calibration to observed data, can bear considerable uncertainty.

For a single model structure, the uncertainty due to model parameters can be estimated using Bayesian methods by conditioning the model behavior on measurements. The literature is replete with methods for uncertainty analysis based on Bayesian formalism, particularly in hydrological studies (e.g. Beven and Binley, 1992). Some Bayesian methods have been applied for uncertainty analysis of crop models. The Generalized Likelihood Uncertainty Estimation (GLUE) method (Beven and Binley, 1992) has been used for the estimation of posterior parameter distributions in studies of wheat using the Simulateur mulTidisciplinaire pour les Cultures Standard (STICS)-wheat model (Varela et al., 2010), sweet corn using the Crop Environment Resource Synthesis (CERES)-Maize model (He et al., 2009), maize and wheat using Root Zone Water Quality Model 2 (RZWQM2) model (Sun et al., 2016), and cotton using the Cropping System Model (CSM)-CROPGRO-Cotton model (Pathak et al., 2012). Despite the computational simplicity and popularity of the GLUE method, concerns about using informal Bayesian likelihood functions in GLUE have been the subject of extensive scientific discourse (Stedinger et al., 2008; Vrugt et al., 2009b).

Alternatively, formal Bayesian methods using Markov-Chain Monte-Carlo (MCMC) techniques have been developed. In crop modeling, MCMC methods have been applied to quantify the uncertainty in predicted phenological development of maize in Slovenia using the World Food Studies (WOFOST) model (Ceglar et al., 2011). More recently, a MCMC method named Differential Evolution Adaptive Metropolis (DREAM) (Vrugt and Ter Braak, 2011) was applied to characterize parameter uncertainties of the STICS model in simulations of winter wheat (Dumont et al., 2014). Another recent study applied the MCMC method with the Systems Approach for Land Use Sustainability (SALUS) model to simulate maize, peanut, and cotton (Dzotsi et al., 2015). The MCMC method was found useful as a method for quantifying uncertainty.

Parameter sensitivity analysis (SA) is usually performed prior to uncertainty analysis to evaluate the importance of model parameters (Ceglar et al., 2011; He et al., 2009; Laloy et al., 2010; Pathak et al., 2012). While several local and global methods are available, global SA methods are more informative since they account for interactions between parameters (Saltelli et al., 2000). Furthermore, global SA can provide information on the structure of the model residuals, which is essential for the implementation of formal Bayesian techniques for uncertainty analysis (Ahmadi et al., 2014).

The DayCent model (Parton et al., 1998) is a widely-used ecosystem model for simulating crop yield, soil carbon, nitrous oxide emissions,

and other agroecosystem responses (Chang et al., 2013; Del Grosso et al., 2006, 2008; Jarecki et al., 2008; Stehfest et al., 2007; Zhang et al., 2013). A few previous studies have assessed the predictive uncertainty of DayCent due to parameter uncertainty (De Gryze et al., 2010; Del Grosso et al., 2010; Fitton et al., 2014; Lee et al., 2011). Two studies, in particular, analyzed the parameter uncertainty on trace gas emissions using Bayesian methods (Van Oijen et al., 2011; Wang and Chen, 2012). The DayCent model is used in widely-deployed decision support systems, including the Carbon Management Evaluation Tool (COMET)--FARM tool (Paustian et al., 2018; <http://cometfarm.nrel.colostate.edu/>; a farm-scale carbon and greenhouse gas accounting tool with new features of water management and water quality in development) and the agroecosystem analysis tool on environmental Resource Assessment and Management System (eRAMS) platform (Arabi, 2011; <https://erams.com/>; a field-to basin-scale water management tool). Thus it is critical to provide accurate uncertainty estimates for crop growth and water dynamics in these tools.

Recent development of the DayCent model include a new crop canopy development algorithm and improved accuracy in predicted crop water use (Zhang et al., 2018b). However, the new crop submodel was manually calibrated and tested for water-limited conditions (Zhang et al., 2018a), leaving a need for a systematic analysis of parameter sensitivity and uncertainty. A systematic analysis could improve our understanding of the model and reveal the weaknesses in model structure (e.g. non-sensitive parameters and constantly biased predictions). Thus, the overall goal of this study was to enhance the applicability of the new version of the model for simulating crop and soil water dynamics under water-limited conditions by analyzing parameter sensitivity and quantifying uncertainty associated with model predictions. Our objectives were to: (i) understand the importance of parameters and the processes they represent in the DayCent model through a global sensitivity analysis; (ii) characterize the uncertainty of important parameters; and (iii) validate the model predictions in water-limited environments.

2. Material and methods

For the sensitivity and uncertainty analysis of the DayCent agroecosystem model (Parton et al., 1998), we used data from a field experiment conducted in Mead, NE which included three treatments: irrigated continuous maize, irrigated maize-soybean rotation, and a rainfed maize-soybean rotation. In our analysis, we first applied Sobol's global sensitivity analysis (Sobol, 1993) to identify the relative importance of model parameters for predicted grain yield, monthly green leaf area index (GLAI), and monthly aboveground biomass. Then results from the sensitivity analysis were used to investigate the structure of model errors using measurement data (six year \times treatment; separated for training and testing). Posterior distributions of the model parameters for one maize hybrid were identified using the DREAM technique. The predictive uncertainty of the training dataset (three out of six year \times treatment combinations) and testing datasets (the remaining three year \times treatment combinations) was estimated.

2.1. Field experiments

Field data were obtained from an experiment conducted at the University of Nebraska Agricultural Research and Development Center near Mead, NE. A detailed experimental design can be found in Suyker and Verma (2009). Although it is not a limited irrigation experiment, the irrigated treatment and rainfed treatments under years with varying amounts of precipitation provide enough information to analyze water stress. The experiment was initialized in 2001. Two of the treatments were irrigated and one was rainfed. Each treatment is a large production field (49–65 ha). One of the irrigated treatments was planted in continuous maize (*Zea mays* L.) (Irrigated Continuous Maize or ICM). The other irrigated treatment was in a maize/soybean (*Glycine max* L.)

Table 1

Crop management for the three treatments of Pioneer 33B51 at Mead, NE.

Treatment/ Year	Plant population (plants ha ⁻¹)	Planting time (DOY ^a)	Harvest time (DOY)	Irrigation and rainfall from planting to harvest (mm)
Irrigated continuous maize (ICM)				
2003	77,000	135	300	629
2004	79,800	125	288	613
Irrigated maize-soybean rotation (IMS)				
2003	78,000	134	296	633
2005	81,000	122	290	636
Rainfed maize-soybean rotation (RMS)				
2001	62,000	134	302	355
2003	57,600	133	286	292

^a DOY is day of year.

rotation (Irrigated Maize-Soybean rotation or IMS). The rainfed treatment was also in a maize/soybean rotation (Rainfed Maize-Soybean rotation or RMS). These treatments weremanaged using standard best management practices in this region for fertilizer, herbicide, and pesticide applications. During the experimental period, different hybrids of maize were grown with different planting date depending on the relative maturity and weather/soil conditions (Zhang et al., 2018b). Hybrid Pioneer 33B51 was planted in 2001, 2003, 2004, and 2005 (Table 1); data from this hybrid were selected for use in this study.

Within each treatment, six 20 × 20 m measurement areas (intensive measurement zones) were established for detailed measurements of leaf area, aboveground biomass, and other important ecosystem variables (Verma et al., 2005). In our study, GLAI, aboveground biomass, and grain yield measurements were the variables of interest. Grain yields were recorded from the measurement of combine harvest of the entire treatment field. Leaf area and aboveground biomass were sampled destructively on an average of 11-day basis at each intensive measurement zone of each treatment.

The soil in all three treatments was a deep silty clay loam with a near level slope. Soil characteristics were measured for four depth increments and details can be found in Zhang et al. (2018b). Air temperature, solar radiation, relative humidity, and wind speed for model simulation were from an on-site weather station (station name MEADAGROFARM; High Plains Regional Climate Center, Lincoln, NE). Precipitation and irrigation amounts needed as model inputs (via a center-pivot irrigation system) were directly measured within each treatment field using rain gauges.

2.2. Agroecosystem model: DayCent

The DayCent ecosystem (cropland, forest, grassland, and savanna) model (Parton et al., 1998), daily version of the CENTURY model (Parton et al., 1987), was used in this study. The major sub-models of DayCent include plant growth, soil water, soil organic matter decomposition, soil nitrogen and trace gas emission. Major inputs for the model are daily weather, soil physical properties, plant type, and management practices. Recently, Zhang et al. (2018b) incorporated a new method to simulate the canopy dynamics of annual crops along with other modifications. The field experiment used in this study has been previously simulated with the improved model using manually calibrated parameters (Zhang et al., 2018b). The results show improved GLAI simulation and a better fit in late season evapotranspiration rate in comparison with the previous version of the model by improving the calculation for green leaf biomass (described later in this section). This version of DayCent has also been applied to simulate limited irrigation experiments in eastern Colorado (Zhang et al., 2018a) with manual calibration.

A brief discussion of the theory, concepts, and methods used in the improved model is presented here. In DayCent, daily potential net primary production is simulated as the product of radiation use efficiency and intercepted photosynthetically active radiation (PAR):

$$PP_i = CC_i \times PAR_i \times RUETB \quad (1)$$

where PP_i is the potential production on the i th day, CC_i is the fraction of radiation intercepted by canopy on the i th day and $RUETB$ is the radiation use efficiency of total biomass production (aboveground and belowground). The variable CC_i is calculated using Beer's Law (Monsi and Saeki, 1953; Sellers, 1985):

$$CC_i = 1 - \exp(-KLIGHT \times GLAI_i) \quad (2)$$

where $KLIGHT$ is the extinction coefficient of vegetation. The actual production is affected by temperature, water, and nutrient. Daily actual production is allocated to above and below-ground based on the development stage and stress (water and nitrogen). Phenology of growth is estimated by a growing degree day (GDD) method. Temperature effect (T_e) on PP_i (approximately a bell-shaped curve) is as follows:

$$T_e = \left(\frac{PPDF2 - T_{mean}}{PPDF2 - PPDF1} \right)^{PPDF3} \times \exp \left\{ \frac{PPDF3}{PPDF4} \times \left[1 - \left(\frac{PPDF2 - T_{mean}}{PPDF2 - PPDF1} \right)^{PPDF4} \right] \right\} \quad (3)$$

where $PPDF1$, $PPDF2$, $PPDF3$, $PPDF4$ are parameters to control the shape of the curve; T_{mean} is the daily mean temperature.

The soil water sub-model simulates 1-dimensional water balance including precipitation, irrigation, evapotranspiration (ET), runoff, and percolation (Parton et al., 1998). Potential ET is simulated by a calculated reference ET and crop coefficients (Allen et al., 1998). Potential ET is partitioned into potential evaporation from the soil and transpiration by the plant, based on GLAI.

Both the crop production sub-model and soil water sub-model require prediction of GLAI. The new GLAI method is described in Zhang et al. (2018b). Briefly, GLAI is converted from green leaf biomass using a constant specific leaf area (SLA). In our new method, green leaf biomass is simulated using green leaf weight ratio (GLWR; as a function of GDD) and aboveground biomass:

$$GLAI_i = AgBiomass_i \times GLWR_i \times SLA \quad (4)$$

2.3. Global sensitivity analysis

Global sensitivity analysis (GSA) apportions the uncertainty in model outputs to the uncertainty in individual inputs and interactions thereof (Saltelli et al., 2000). The 'Sobol' method is arguably the most comprehensive GSA method due to its sampling design for the exploration of the parameter space. The decomposition of the variance of the model outputs $Var(\hat{Y})$ for k parameters (θ) is written as:

$$var(\hat{Y}) = \sum_{i=1}^k D_i + \sum_{1 \leq i < j \leq k} D_{ij} + \dots + D_{1\dots k} \quad (5)$$

where D_i is the main effect of input parameter θ_i . The terms of $D_{ij}, \dots, D_{1\dots k}$ correspond to the interactions between parameters. The computation of these terms can be found in Sobol (1993) and is not discussed here.

The sensitivity indices are given by:

$$S_{i_1, \dots, i_s} = D_{i_1, \dots, i_s} / var(\hat{Y}) \quad (6)$$

where $1 \leq i_1 < \dots < i_s \leq k$ and $s = 1, \dots, k$. Hence, the first-order sensitivity indices (main effects) for each parameter are:

$$S_i = D_i / var(\hat{Y}) \quad (7)$$

Total order indices are then computed as:

$$TS_i = S_i + \sum_{1 \leq i < j \leq k} S_{ij} + \dots + S_{1\dots k} \quad (8)$$

Table 2

The input parameters for the sensitivity analysis.

Name	Definition	Unit	Lower bound	Upper bound	Reference number	Reference
Growth and production						
RUETB	Radiation use efficiency for total biomass production	$\text{g m}^{-2} \text{ langley}^{-1} \text{ PAR}$	0.12	0.2	1	Zhang (2016)
PPDF1	Optimal temperature for production	(°C)	25	32	2	Necpálová et al. (2015) and Zhang et al. (2018b)
PPDF2	Maximum temperature for production	(°C)	35	50	3	Necpálová et al. (2015) and Zhang et al. (2018b)
DDEMERG	GDDs from planting to emergence	Degree-day	50	120	4	Field measurement
DDBASE	GDDs from planting to anthesis	Degree-day	600	900	5	Field measurement
MXDDHRV	The maximum number of degree days from anthesis to harvest	Degree-day	650	850	6	Field measurement
GAPMNDD ^a	The difference between MNDDHRV and MXDDHRV	Degree-day	0	600	7	Field measurement
BMINI	Initial biomass at emergence	g m^{-2}	0.1	2	8	Field measurement
SLA	Specific leaf area	$\text{m}^2 \text{ g}^{-1}$	0.015	0.025	9	Field measurement
LEAFEMERG	Intercept of the second stage linear equation at emergence	g g^{-1}	0.8	0.95	10	Field measurement
LEAFMX	Green leaf weight ratio at maximum GLAI	g g^{-1}	0.2	0.35	11	Field measurement
LEAFPM	Green leaf weight ratio at physiological maturity	g g^{-1}	0	0.1	12	Field measurement
FRTC1	Fraction of C allocated to roots at planting, with no water or nutrient stress,	g g^{-1}	0.3	0.5	13	Developers' suggestion
FRTC2	Fraction of C allocated to roots when reaches maximum root depth	g g^{-1}	0.05	0.2	14	Developers' suggestion
FRTC3	Time after planting at which the FRTC2 value is reached	days	70	110	15	Developers' suggestion
FRTC4	The maximum increase in the fraction of C going to the roots due to water stress	g g^{-1}	0.01	0.3	16	Developers' suggestion
HIMAX	The maximum harvest index	g g^{-1}	0.5	0.6	17	Field measurement
HIWSF	Water stress factor on harvest index	–	0.3	0.7	18	Developers' suggestion
KLIGHT	Extinction coefficient of Beer's Law	–	0.4	0.8	19	Developers' suggestion
ET and soil water						
KCET	Crop coefficient for evapotranspiration	–	0.9	1.3	20	Allen et al. (1998) and Suyker and Verma (2009)
dmpflux	The damping factor for soil water flux is a multiplier used to reduce (or dampen) the upward and downward soil water fluxes between two soil layers in a Darcy's Law calculation.	–	1E-7	1E-5	21	Developers' suggestion
BD	Bulk density	g m^{-3}	1.3	1.5	22	USDA NRCS ^b
P _{sand}	Sand content	–	0.05	0.2	23	USDA NRCS
P _{clay}	Clay content	–	0.27	0.4	24	USDA NRCS

^a GAPMNDD is not a real parameter in the model. MNDDHRV is the minimum number of degree days from anthesis to harvest.^b USDA Natural Resources Conservation Service soil texture triangle.

Twenty-four parameters in the improved version of DayCent model were used in sensitivity analysis (Table 2). These parameters can be divided into two groups: i) crop growth/production related parameters, which are species or cultivar specific; and ii) parameters representing ET and soil water processes. Uniform distributions were assumed for the prior parameter distributions (DeJonge et al., 2012; Dzotsi et al., 2015). The ranges of model parameters were selected based on field measurements at the Mead site and/or relative studies in the literature.

Global sensitivity analysis using the method of Sobol requires independence of parameters. However, parameters *MNDDHRV* (minimum number of degree days from anthesis to harvest) and *MXDDHRV* (maximum number of degree days from anthesis to harvest) are not independent (*MNDDHRV must be smaller than MXDDHRV*). A new parameter *GAPMNDD*, the difference between *MNDDHRV* and *MXDDHRV*, was defined as a random variable. *MNDDHRV* was then calculated based on the *MXDDHRV* and *GAPMNDD*. Additionally, a wider range of 0.9–1.3 for the crop coefficient for evapotranspiration (*KCET*) parameter was used because field measurements indicated smaller values (1.03 ± 0.07 , Suyker and Verma, 2009) than those reported by Food and Agriculture Organization of the United Nations (FAO) (Allen et al., 1998). Soil parameters including saturation point, field capacity, wilting point, and saturated conductivity were estimated by soil texture using the Saxton equation (Saxton et al., 1986). The sand content, clay content, and bulk density were varied within the ranges of a silty clay loam (U.S. soil texture triangle) by assuming only one soil texture in the experimental fields. Soil parameters were inputs to the model and were not changed during the simulation. The model sensitivity to input weather variables were not included in this study; it was analyzed and published previously (Zhang and Paustian, 2019).

In this study, a sample size of 25,600 was generated using the SimLab software (Joint Research Center of the European Commission, 2004). This sample size meets the requirement of $n \times (k+2)$ (with n in range of 500–1000 typically; k is the number of parameters) to ensure numerical stability (Saltelli et al., 1999, 2005). These samples of parameter sets were used to run the simulations for hybrid Pioneer 33B51 (total six year \times treatment; Table 1). The model responses examined in the sensitivity analysis were annual grain yield, monthly aboveground biomass, and monthly GLAI. Monthly averages of aboveground biomass and GLAI in May, July, and September were examined for differences in sensitivity during early, middle, and late growing seasons, as the timing of drought stress is important for crop development.

Important model parameters were then included in parameter and predictive uncertainty analysis. The criterion for classifying parameters as “important” was sensitivity indices greater than 0.05 for monthly aboveground biomass, monthly GLAI, or annual grain yield.

2.4. Bayesian parameter uncertainty analysis using DREAM

Using Bayesian formalism, the posterior distribution (Π) of a set of parameters θ of model responses (\hat{Y}) conditioned on observed data Y is:

$$P(\theta|Y) = \frac{P(Y|\theta) P(\theta)}{\int P(Y|\theta) P(\theta) d\theta} \quad (9)$$

where $P(Y|\theta)$ represents the likelihood of the data, $P(\theta)$ is the prior distribution of parameters. The likelihood $P(Y|\theta)$ is determined from the probability distribution of the residuals between observed (Y) and modeled (\hat{Y}) responses. Residuals are often assumed to be uncorrelated,

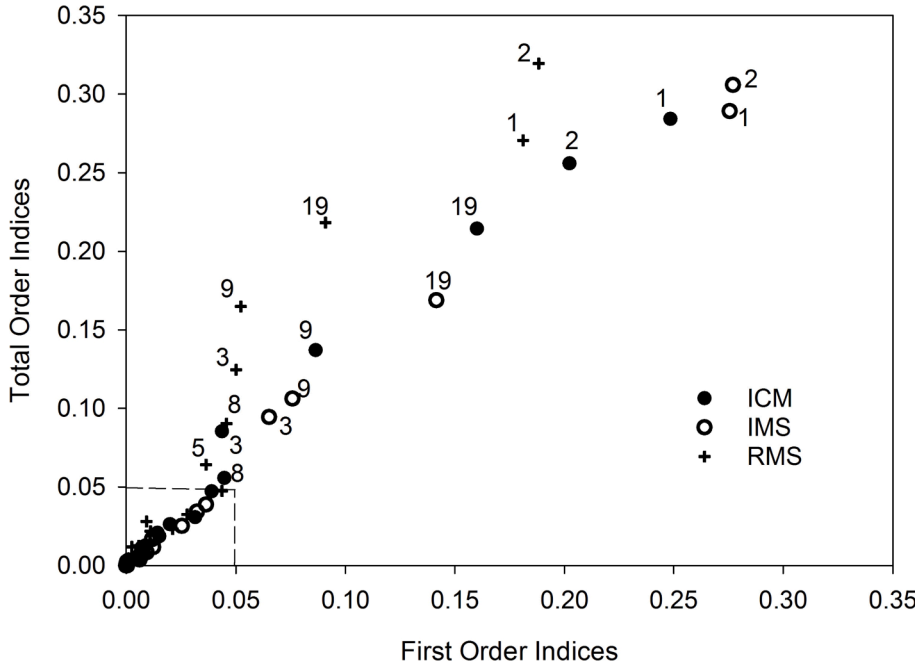


Fig. 1. Comparison of first order and total order sensitivity indices of Sobol for DayCent output of grain yield of maize from three treatments. Treatments were irrigated continuous maize (ICM), irrigated maize-soybean (IMS) and rainfed maize-soybean (RMS). The numerical values are references to parameters in Table 2. Dashed line indicates the criterion for selection of important parameters. A zoom-in view of this figure focusing on the index values less than 0.05 is Fig. A2 in the Appendix.

independent, normally distributed (Box and Tiao, 1992), hence yielding the likelihood function:

$$L(\theta|Y) = \prod_{i=1}^n (2\pi\sigma_e^2)^{-1/2} \times \exp\left(-\frac{1}{2\sigma_e^2} [\hat{Y}_i(\theta) - Y_i]^2\right) \quad (10)$$

where σ_e is the standard deviation of model errors and n is the number of observed responses. Assuming homoscedastic model residuals, the log likelihood function is:

$$L(\theta|Y) = -\frac{n}{2} \ln(2\pi) - 2n \ln(\sigma_e) - \frac{1}{2\sigma_e^2} \sum_{i=1}^n [Y_i - \hat{Y}_i(\theta)]^2 \quad (11)$$

When model residuals are not homoscedastic, observed and model responses are typically transformed using appropriate transformations, e.g. Box-Cox transformation (Box and Cox, 1964), prior to computation of the likelihood function. Similarly, autoregressive time series models, e.g. first-order autoregressive transformation (AR-1), may be applied to remove model error autocorrelation (Ahmadi et al., 2014; Vrugt, 2016).

MCMC simulations are commonly used for estimation of posterior parameter distributions as a formal Bayesian method. The DREAM algorithm (Vrugt et al., 2008, 2009a; Vrugt and Ter Braak, 2011; Vrugt, 2016) was selected for this study. The advantage of this approach is its efficiency in mitigating issues with high-dimensionality, multimodality, nonlinearity, and local optima with proved ergodicity compared with some traditional MCMC algorithms. Vrugt (2016) presents a complete review of the theory, concepts, and MATLAB implementation for the DREAM approach.

2.5. Identification of the structure of model residuals

DayCent model residuals were investigated for homoscedasticity, normality, and uncorrelated residuals. From the 25,600 GSA runs, outputs were extracted and residuals were calculated for each run using measurement data of annual grain yield, multiple in-season GLAI measurements and in-season aboveground biomass of hybrid Pioneer 33B51. Residuals for the “best” model parameters, selected based on the minimum root mean squared error (RMSE), were explored. Model residuals of the three response variables (i.e., yield, GLAI, biomass) were examined for heteroscedasticity using the chi-square test for normality. Since the GLAI and biomass are only continuously measured within each year,

partial autocorrelation in each year was also graphically assessed.

2.6. Implementation of the DayCent linkage with DREAM

The R package for DREAM (Guillaume and Andrews, 2012) was integrated with the DayCent model to conduct the parameter uncertainty analysis. We wrote a script in R to compute the likelihood function required as input to the DREAM package. Twelve MCMC chains were used in this study. The Gelman and Rubin (1992) statistic (\hat{R}) of 1.2 was used for convergence. The first 50% of simulations were treated as the so-called burn-in runs (discarded) after which chain approached its stationary distribution (Vrugt and Ter Braak, 2011).

The measurement data used in residual analysis were divided into two datasets for training and testing. Data from the ICM treatment in 2004, IMS treatments in 2005, and RMS treatment in 2001 were used for training since these data covered variations in planting dates, water stress (irrigated vs non-irrigated), and growing season temperature. This data set contained 28 measurements of GLAI, 26 measurements of aboveground biomass, and 3 measurements of annual grain yield. For testing purposes, measurements from the three treatments in 2003 were used. The measurement data included 24 measurements of monthly GLAI, 24 measurements of monthly aboveground biomass, and 3 measurements of annual grain yield.

The σ_e in Equation (11) is associated with uncertainty. The σ_e values were estimated in parallel with the DayCent parameters (Iizumi et al., 2014). Very wide uniform prior distribution was used for σ_e for grain yield (sigma_GrainCarbon, 10–200 g C m⁻²; grain carbon is a good predictor for corn yield but may not be for other crops), aboveground biomass (sigma_AbovegroundCarbon, 10–400 g C m⁻²), and GLAI (sigma_GLAI, 0.1–2.5). The predictive uncertainty for GLAI, aboveground biomass, and annual grain yield were computed using the last 10% of parameter sets from the DREAM algorithm after convergence.

2.7. Uncertainty in the prediction of crop water production functions

We used input variables from the rainfed treatment at Mead for a 12-year period from January 2001 to December 2012 to generate crop production functions. Only the dry years in this period (2001, 2003, and 2012) were in our analysis to show the drought effect on production.

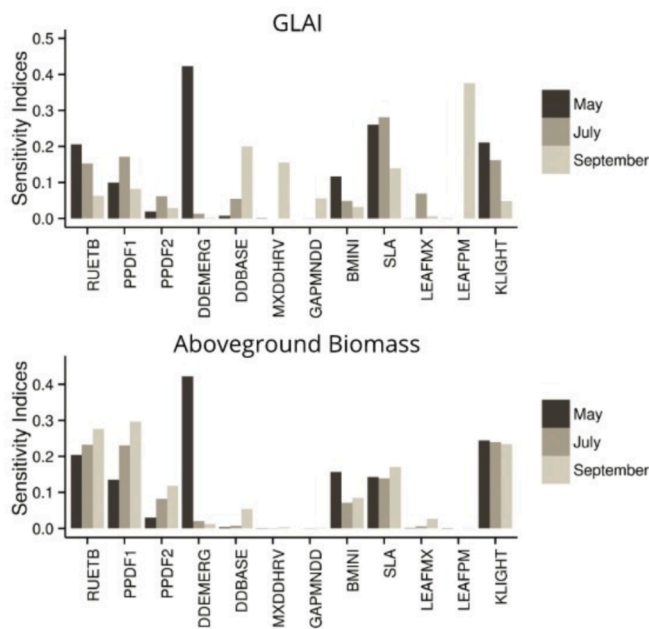


Fig. 2. Total sensitivity indices for DayCent output of green leaf area index (GLAI) and aboveground biomass in May, July, and September representing early, middle, and late growing season, respectively. Only input parameters with total sensitivity indices higher than 0.05 in at least one month were shown.

The planting date was fixed at DOY 130. Simulations were then conducted assuming no nutrient stress to be able to discern the effects of water stress at varying irrigation levels. Evidences showed interactions of moisture stress and nutrient uptake by corn and other crops (Ahanger et al., 2016; Ahmad et al., 2014; Eissa and Roshdy, 2019) but this synergistic effect is beyond the model's capability and was not considered in this study.

The optimal DayCent parameter set from DREAM computational experiments was used to estimate irrigation requirements to meet crop consumptive use in each year within the analysis period. Subsequently, the uncertainty of model responses was evaluated for limited irrigation treatments at 0 (i.e. rainfed), 20, 40, 60, and 80 percent of full irrigation requirements.

3. Results and discussion

3.1. Important DayCent parameters and critical crop growth processes

Fig. 1 presents a summary of the main effects (first order indices) and total effects (total order indices) of DayCent model parameters on the estimated average annual grain yield for the ICM, IMS, and RMS treatments. The most important parameters were crop growth/production related parameters. The total sensitivity indices for ET and soil water related parameters were very small even under rainfed treatment (RMS).

Parameters *PPDF1*, *RUETB*, and *KLIGHT* were the most important parameters for all treatments. Results suggest that more attention should be paid to the optimum temperature for production (*PPDF1*). Radiation use efficiency (*RUETB*), the primary parameter that controls the potential crop growth in DayCent, was found to have a very high sensitivity index. These results corroborate findings for other crop models with similar scientific theory and conceptualization for crop growth simulation, including CERES-Maize (DeJonge et al., 2012) and EPIC (Wang et al., 2005). The extinction coefficient parameter (*KLIGHT*) is another parameter widely used by crop models which determines how much light can be intercepted by the canopy for photosynthesis; thus it is expected to be very influential on yield (Pathak et al., 2007).

Results indicated that variation in the soil texture parameters (*BD*, *P_{sand}*, and *P_{clay}*) within a given texture class had a relatively small influence on simulated average annual crop yields, which justifies the use of generalized soil texture classes in regional studies, or field level studies where detailed soil information are not available. Similarly, soil property parameters used in CERES-Maize were found to have relatively low sensitivity for prediction of grain yield of corn in both full and limited irrigation treatments (DeJonge et al., 2012). Ma et al. (2009) showed relatively large variation of the saturated conductivity (*K_{sat}*) of soils with high percent of sand could result in significant change in crop yield in crop simulations. In our simulation, *K_{sat}* was predicted by the Saxton pedotransfer equation based on soil texture. The small predicted *K_{sat}* and its relative small range for silty clay loam (0.00008–0.0003 mm/h) resulted in limited impact on yield. The *KCET* (crop coefficient for ET) parameter in the rainfed treatment was more important than for the two irrigated treatments. This result is plausible since higher potential ET rate (higher *KCET* value) results in higher actual ET and subsequently higher drought stress when irrigation is not available to mitigate water stress (the impact is crop type and growth stage dependent).

The sensitivity of seasonal or monthly crop response variables in DayCent has not been investigated in previous studies. As the timing of drought stress within the growing season is important in crop development (Jha et al., 2018; Saseendran et al., 2014), we presented the total sensitivity indices for May, July, and September in the rainfed treatment, corresponding to early, middle, and late growing season (Fig. 2). Better understanding of within season variation in stress responses is vital for proper parameterization of models in response to temporal variability of climatic conditions. Results are depicted only for parameters with indices greater than 0.05 for monthly GLAI and aboveground biomass. The ranking of indices of the two irrigated treatments is similar except for the parameter *GAPMND*, which was more important in the rainfed treatment since it represents the change of GDD requirement from anthesis to maturity under drought stress. The three most important parameters for grain yield (*PPDF1*, *RUETB*, and *KLIGHT*) were also important in most months for GLAI and aboveground biomass. In some months, a single DayCent parameter was shown to be most influential. For example, in May, the sensitivity indices for *DDEMERG* for both GLAI and aboveground biomass were higher than 0.4, showing the large sensitivity of early crop growth to parameters controlling time of emergence after planting.

3.2. Analysis of residuals from sobol GSA

Model residuals for the GSA simulation with the lowest RMSE were analyzed to identify a proper likelihood function for uncertainty analysis (Appendix Fig. A1). Heteroscedasticity was not detected in model residuals using the Brown-Forsythe test (*p* values for GLAI and biomass were 0.246 and 0.462, respectively). The homoscedasticity of grain yield residuals was not tested because only six observations were available. Residuals for all three responses (monthly GLAI, monthly aboveground biomass, and annual grain yield) were normally distributed, based on the chi-square test for normality at 0.05 significance level (*p* values for GLAI, biomass, and grain yield were 0.918, 0.088, and 0.059, respectively). The partial autocorrelation plots of each year and treatment showed no significant correlation at any lag.

3.3. Posterior distribution of parameters

The DREAM algorithm does not only predict the best value for a parameter but also the statistical distribution of each parameter value as informed by the measurements. The marginal posterior probability density function (PDF) for the 12 most important DayCent parameters and three σ_ϵ from DREAM were plotted (Fig. 3). The summary of the basic statistics and the optimal value for each parameter are shown in Table 3. The *RUETB*, *PPDF1*, *DDEMERG*, *DDBASE*, *BMINI*, and *KLIGHT*

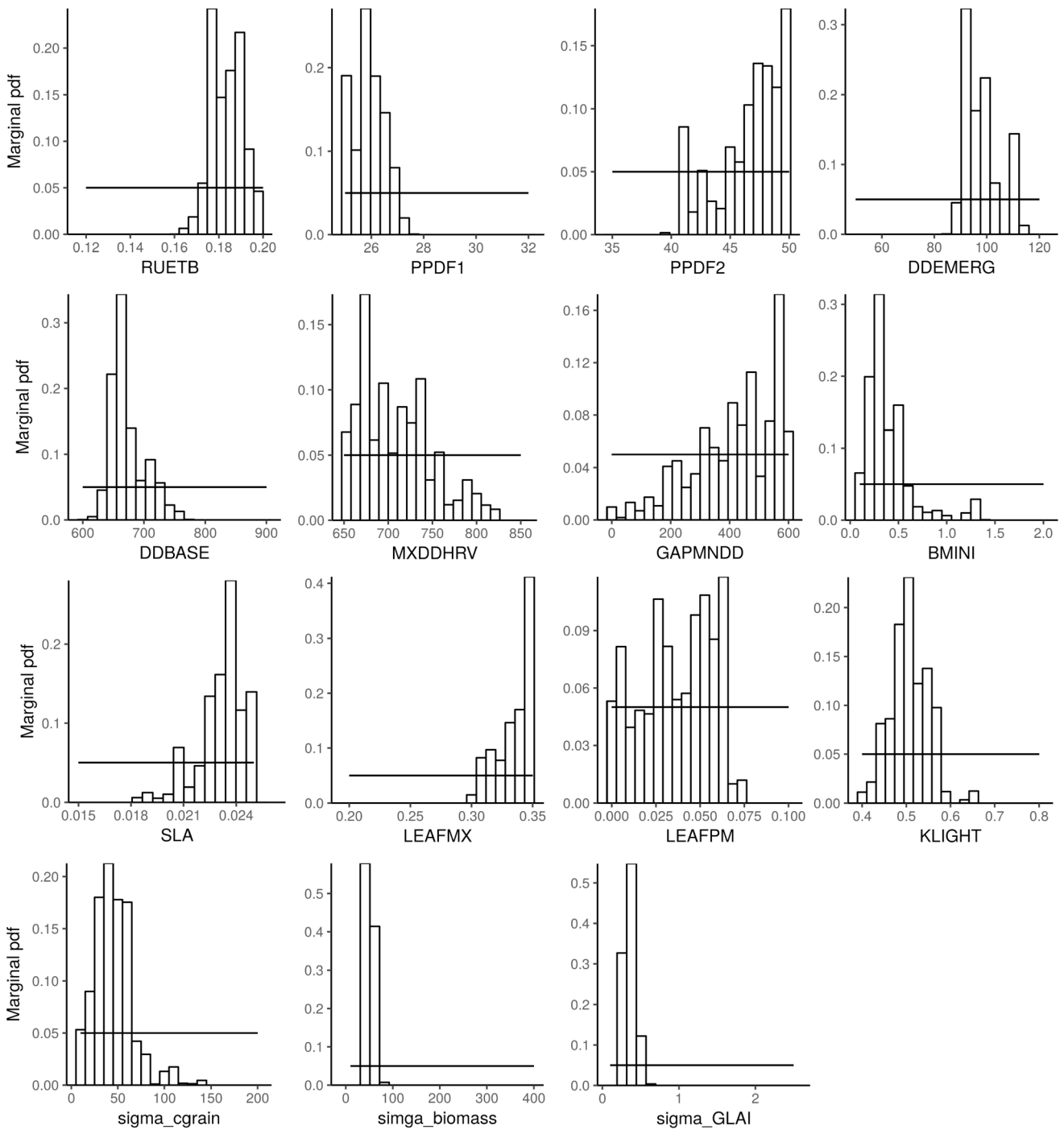


Fig. 3. The marginal probability density functions (pdf) of the parameters used in DREAM algorithm. The horizontal solid line indicates the prior distribution of the parameters.

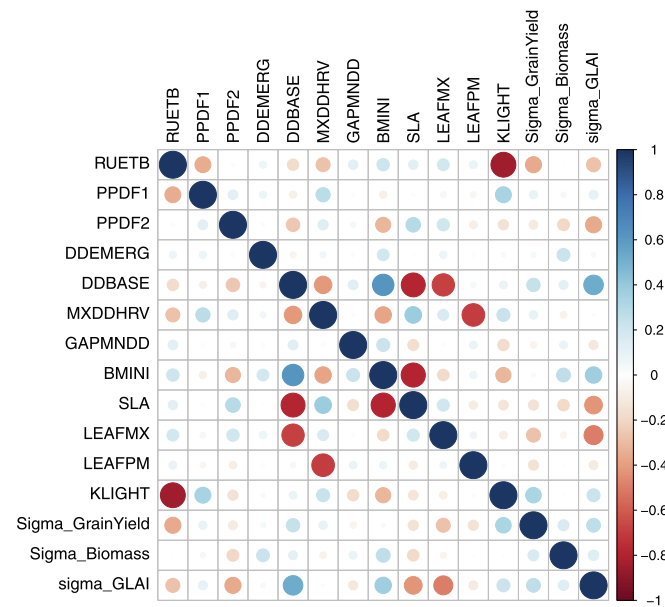
parameters exhibited approximately normal or log-normal distributions, suggesting that the central tendency and variability of the parameters were well defined by the measurements. For MXDDHRV, GAPMND, LEAFPM, the most likely values were not well informed by the measured data as the shapes of the posterior distributions were close to a uniform distribution. PPDF2 and LEAFMX exhibited their highest probability at their upper bounds despite the fact that the full range between upper and lower bounds represent reasonable limits in field observations. Both of them were curve defining parameters in the model (the temperature response curve defined by Equation (3) and the curve of *GLWR* which is used in Equation (4)), suggesting the model structure in simulating these responses can be improved.

Fig. 4 illustrates the correlation structure between posterior parameters from DREAM analysis. A strong negative correlation was evident between *RUETB* and *KLIGHT*. This observation can be explained because to produce the same amount of biomass when more light is intercepted (i.e. greater *KLIGHT*) the radiation use efficiency would have to decrease (i.e. smaller *RUETB*). A high negative correlation was also found between *DDBASE* and *LEAFMX*. When the time of maximum *GLAI* is delayed, the *LEAFMX* (*GLWR* at maximum *GLAI*) decreases because of the linear function with negative slope used in the revised DayCent model (Zhang et al., 2018b). The *DDBASE* parameters was also highly correlated with *SLA* as they control the leaf biomass and *GLAI* (an increase in *DDBASE* or *SLA* results in higher *GLAI*). For highly correlated

Table 3

Summary of the statistics of parameter uncertainty analysis.

Parameter	Optimal	Mean	SD
RUETB	0.183	0.184	0.00764
PPDF1	26.0	25.8	0.651
PPDF2	48.2	46.7	2.54
DDEMERG	92.5	96.3	5.63
DDBASE	659	677	30.7
MXDDHRV	794	736	46.7
GAPMNDD	564	442	148
BMINI	0.352	0.580	0.463
SLA	0.0248	0.0228	0.00169
LEAFMX	0.346	0.337	0.0114
LEAFPM	0.00839	0.0240	0.0183
KLIGHT	0.447	0.495	0.0625
sigma_GrainCarbon	49.6	49.6	25.8
sigma_AbovegroundCarbon	42.3	48.9	7.89
sigma_GLAI	0.281	0.352	0.0694

**Fig. 4.** The correlation of the parameters from the analysis using DREAM algorithm.

parameters, the value of one parameter affects how we choose the correlated parameters; and the posterior distribution of a parameter cannot be seen as separate from the other parameters. For predictive uncertainty analysis, it is not right to generate samples from the posterior distributions without considering their correlations. The correlations between other parameters in Fig. 4 were relatively low.

3.4. Predictive uncertainty for the training data

We first used the optimal parameter set from DREAM to generate predictions for the training dataset and compared model results with field observations. The optimal parameter values provided optimized predictions for biomass with $\text{RMSE} = 979.9 \text{ kg ha}^{-1}$ and $R^2 = 0.98$ (Fig. 5). The predictions for GLAI was slightly lower ($\text{RMSE} = 0.79$ and $R^2 = 0.84$). There was substantial underestimation of GLAI at the late growing season for IMS in 2005 (Fig. 5). This suggested the phenology was not predicted correctly, because the onset and the end of leaf senescence were controlled by phenology. This was also suggested by the wide and flat posterior distributions of MXDDHRV, GAPMNDD, and LEAFPM (i.e., the algorithm could not find a well-defined, small range for these parameters that relate to phenology and leaf senescence), which indicates that the model structure needs improvement. One

possible improvement could be to calculate heat units hourly instead of daily and use non-linear temperature functions (Yin and Laar, 2005). Regarding the grain yield, it was accurately predicted using the optimal parameter values ($\text{RMSE} = 514.8 \text{ kg ha}^{-1}$ and $R^2 = 0.92$).

The DREAM algorithm predicted relative narrow 95% uncertainty bands for the training dataset (Fig. 5) but with several observations outside the bands. Similar results were found in Dumont et al. (2014) which also used the DREAM algorithm for predictive uncertainty analysis. The narrower uncertainty bands were because only parameter uncertainty was included in our analysis; input uncertainty and model structural uncertainty would be needed to characterize total uncertainty and expand the uncertainty band (Ajami et al., 2007).

3.5. Predictive uncertainty for the testing data

For the testing dataset, the optimal parameter values yielded accurate prediction for biomass ($\text{RMSE} = 1575.2 \text{ kg ha}^{-1}$ and $R^2 = 0.96$) but the accuracy was lower than for the training dataset, as expected (Fig. 6). Similarly, the accuracy for GLAI was lower ($\text{RMSE} = 1.06$ and $R^2 = 0.78$). The GLAI of the two irrigated treatments (ICM and IMS) was under-predicted for the whole growing season which may be because the days to anthesis were under-predicted. Corn is generally believed to have very low sensitivity to photoperiod (Corbeels et al., 2016; Soltani and Sinclair, 2012); however, some cultivars might respond significantly as demonstrated by CERES-Maize model studies (DeJonge et al., 2012; Saddique et al., 2019). Including photoperiod responses in our simulation might produce better predictions of days to anthesis. The water stress effect for the rainfed treatment RMS was not very well estimated and led to an over-prediction of biomass, GLAI and grain yield at harvest (Fig. 6). The RMSE for grain yield (999.5 kg ha^{-1}) was lower than the training data but the R^2 (0.96) was slightly higher. The width of the 95% uncertainty bands were similar to the training data. The overall accuracy was high considering the large variation across the large experimental fields (49–65 ha per field). In one of our previous studies, the model was able to accurately simulate water stress effect for corn under various water stressed conditions at different locations in Colorado (Zhang et al., 2018a). The reason for the overestimation for the rainfed treatment here was found to be the inaccurate estimation of soil water (Fig. A3). This could be a result of the uncertainty in precipitation and/or soil properties due to spatial variability across such large fields.

3.6. Prediction uncertainty interval for crop water production functions

For each irrigation scenario during the three driest years (2002, 2003, and 2012; annual precipitation less than 60 cm), distributions of predicted yields were plotted using a boxplot (Fig. 7). The response of yield to irrigation was very clear. The median values of predicted yield of the non-irrigated scenario were about half of those of the full irrigation scenario in these years. Irrigation level of 80% ET replacement was predicted to produce similar yields as the 100% scenario. This is supported by our understanding from field studies (e.g. English, 1990) that the increase in yield slows down when irrigation increases towards meeting total crop water demand. We also observed that the coefficient of variation (CV) of predicted yields, which is a standardized measure of dispersion of a distribution, at every irrigation level was within a narrow range (0.05–0.13). Similar to our work, posterior distributions of parameters can be easily used to generate uncertainty estimates of crop production functions for other locations and other crops or cultivars. These crop production functions will be site-specific and in theory more accurate than a generalized crop production function for a larger region. Using climate models to generate future weather as an input, site-specific predictions could be made for assessing crop responses to climate change which could support decision making for farmers and irrigation managers. Our uncertainty analysis can be extended to provide uncertainty estimates for decision supporting tools such as COMET-FARM and the eRAMS system, which run the DayCent model as part

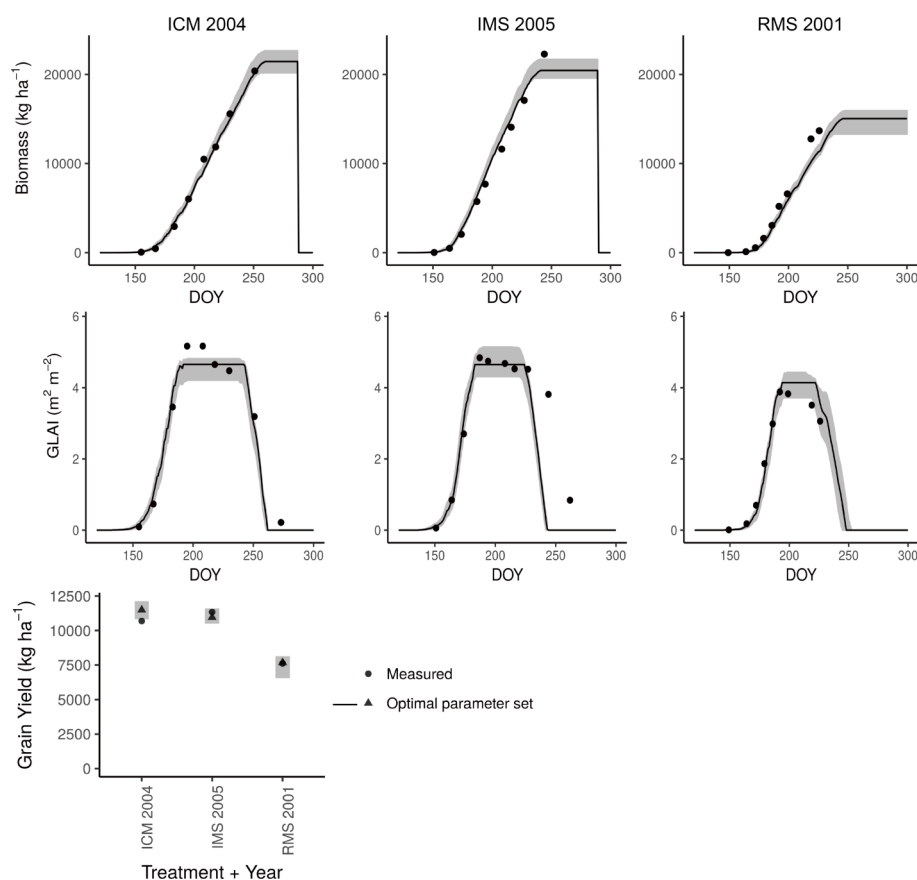


Fig. 5. Comparison of predictive 95% uncertainty (gray band) with measured data (dots) of the calibration dataset of aboveground biomass, GLAI and grain yields for 3 treatments in 3 years.

of their predictive functions.

3.7. Limitations

We quantified predictive uncertainty due to parameter uncertainty in this study. Uncertainty from input forcing (e.g. weather variables) can be added to the analysis by providing prior distributions of multipliers of these variables (it is impossible to set prior distribution for each daily value) (Vrugt et al., 2008). For future predictions, it is popular to use an ensemble approach, which uses more than one climate datasets to drive an agro-ecosystem model (e.g. Baigorria et al., 2008). The quantification of structural uncertainty is difficult. Engeland et al. (2005) estimated the total of parameter uncertainty and structural uncertainty by adding the model residuals to each of the output values at each step of the MCMC algorithm. However, we agree with Marshall et al. (2007) that a robust way of estimating structural uncertainty requires multiple models. The outputs from multiple models are used to generate an ensemble. The Bayesian Model Averaging method (Fragoso et al., 2018) is popular in this category. We will address the uncertainty from input forcing and model structure in future studies.

4. Conclusions

In this study, we analyzed the sensitivity and uncertainty of DayCent model parameters for one hybrid of corn growing in well-irrigated versus water-stressed treatments. We also quantified the predictive uncertainty of simulated grain yield for varying degrees of water stress. We found that among the 24 parameters tested, the growth/production related parameters in DayCent had relatively more impact on grain yield, GLAI, and biomass than did ET and soil water related parameters, for both rainfed and irrigated conditions. Under rainfed conditions,

evapotranspiration related parameters and drought stress related parameters showed higher sensitivity than irrigated conditions as expected. Our monthly results demonstrated that the sensitivity could be highly dependent on the seasonality. As most of the model parameters have physiological meanings, the sensitivity results implied that breeding and selecting cultivars for traits that have the greatest sensitivity/impact on growth could substantially improve production under both irrigated and non-irrigated conditions. These could include cultivars with better heat tolerance, higher capacity of light utilization, and canopy structures that allowing higher planting density. For dryland crops, cultivars with lower transpiration potential would be more drought tolerant and potentially produce more yield. Our analysis also revealed some model weaknesses for future improvements.

In addition, our study provides a rigorous template for producing crop water production functions with well-defined uncertainty bounds that can be used to provide management recommendations to improve the water use efficiency of annual crop production. For our study conditions, the results suggested that 80% of full irrigation could lead to similar grain yield as for full irrigation in dry years, which could help farmers to save water without losing yield. The relative narrow uncertainty band indicated that agro-ecosystem models can be reliable in producing estimates for decision-making. Similar simulations with predictive uncertainty can be made for different crops and locations to provide improved information for water management.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

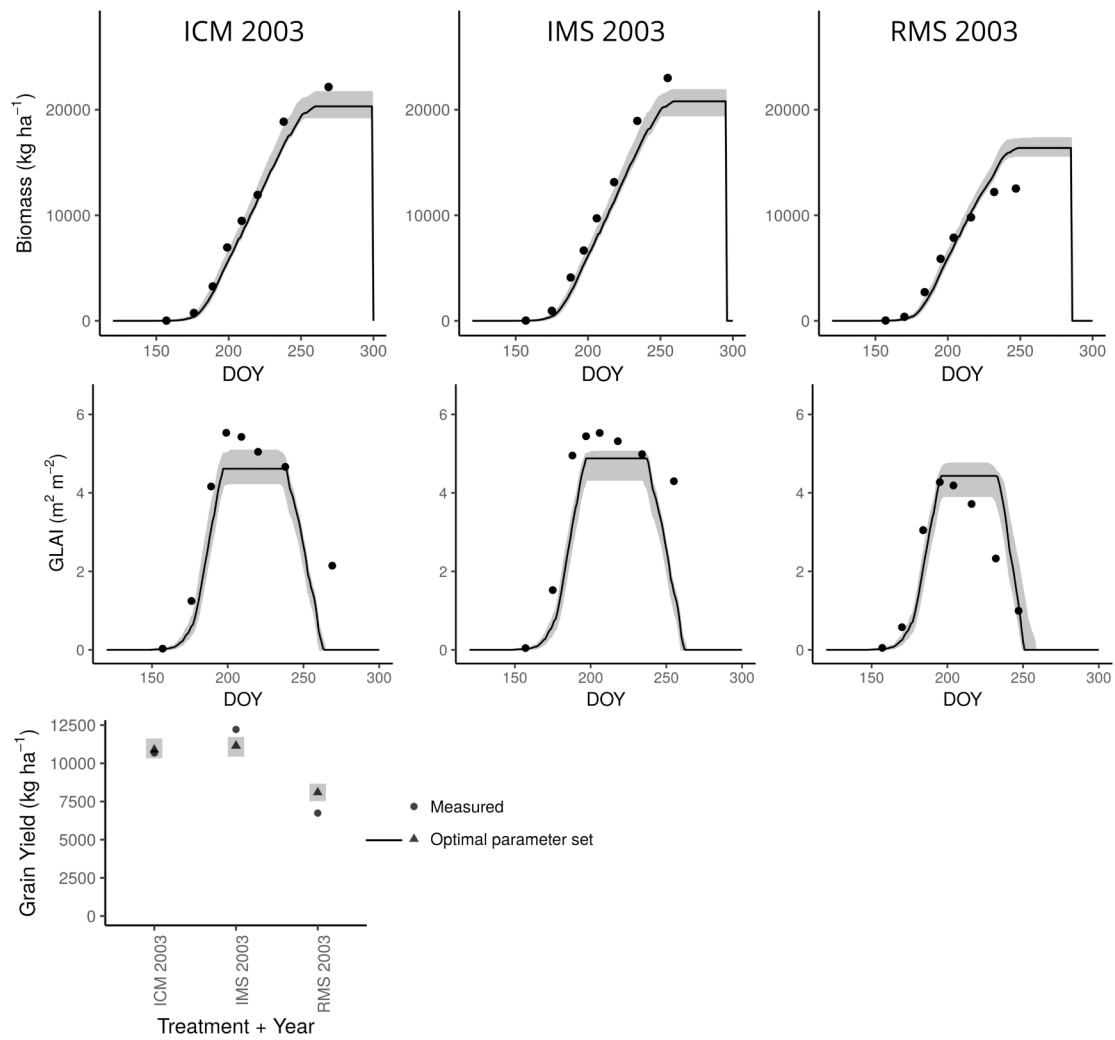


Fig. 6. Comparison of predictive 95% uncertainty (gray band) with measured data (dots) of the validation dataset of aboveground biomass, GLAI and grain yields for 3 treatments in 3 years.

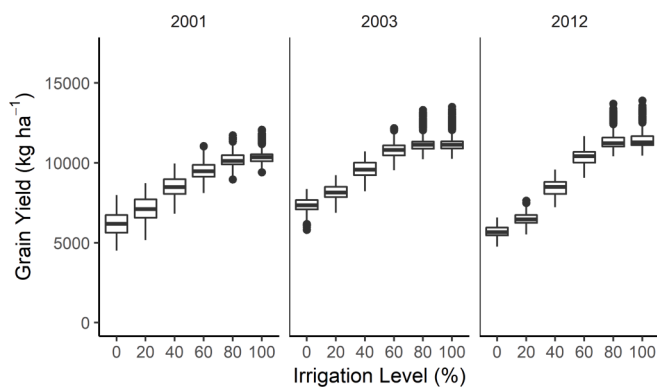


Fig. 7. The box plots of the predicted grain yield using parameter sets from DREAM algorithm for six irrigation levels (percentage of the 100% full irrigation scenario) for 3 years at Mead, NE.

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A. Appendix

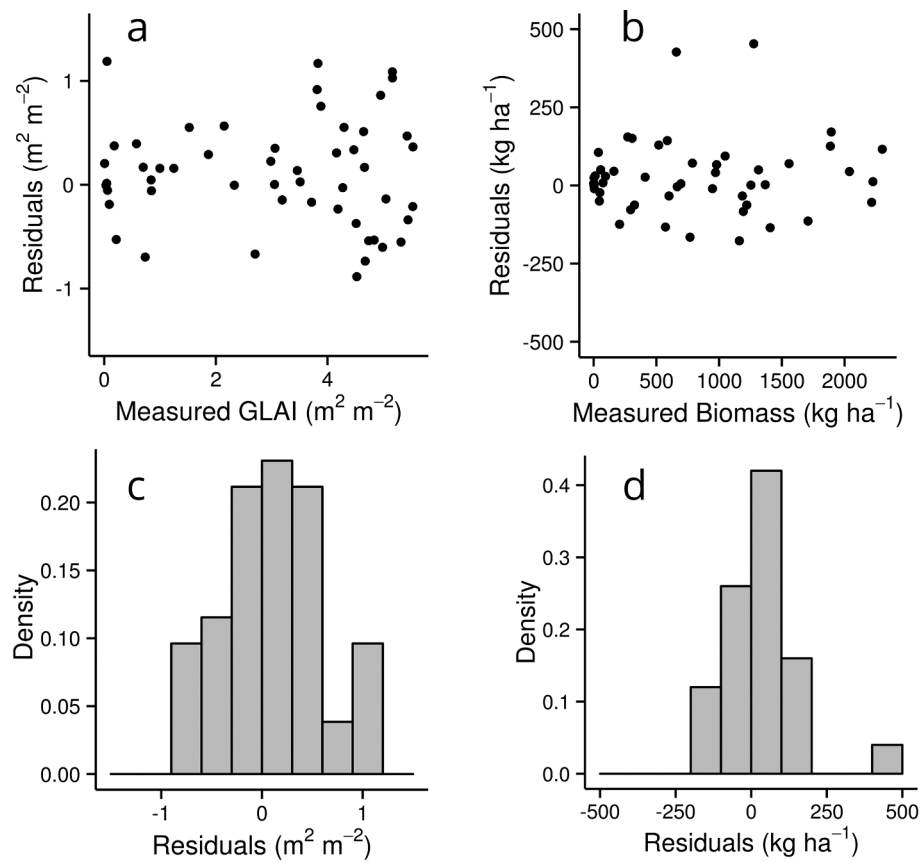


Fig. A1. Modeled residuals plotted against a) measured GLAI and b) measured aboveground biomass. The density plots of residuals are for c) GLAI and d) aboveground biomass.

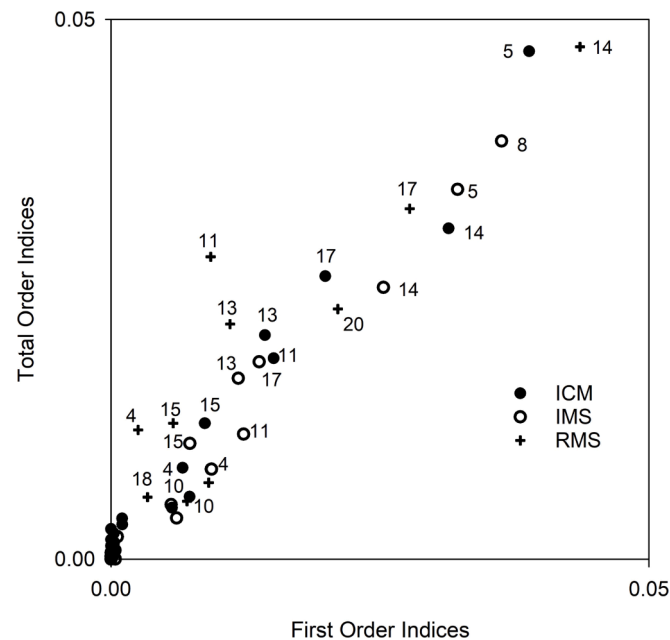


Fig. A2. Zoom-in view of Fig. 1 ($x < 0.05$ and $y < 0.05$). Comparison of first order and total order sensitivity indices of Sobol for DayCent output of grain yield of maize from three treatments. Treatments were irrigated continuous maize (ICM), irrigated maize-soybean (IMS) and rainfed maize-soybean (RMS). The numerical values are references to parameters in Table 2.

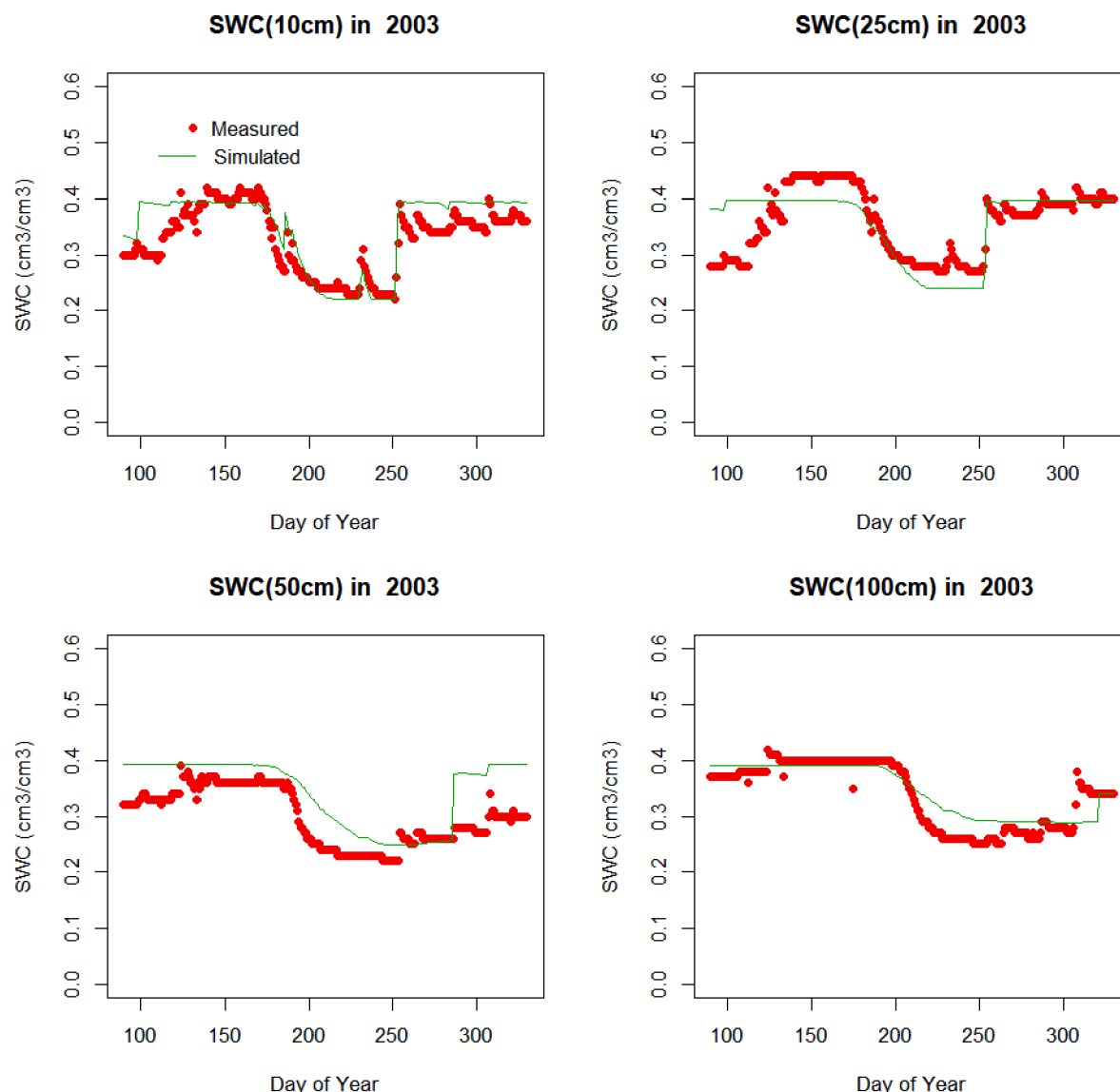


Fig. A3. Simulated and measured soil water content (SWC) of the RMS treatment in 2003. The over-estimation of SWC at 50 and 100 cm resulted in the over-estimation of biomass and yield in Fig. 6 for the RMS treatment.

References

- Ahanger, M.A., Morad-Talab, N., Abd-Allah, E.F., Ahmad, P., Hajiboland, R., 2016. Plant growth under drought stress. In: *Water Stress and Crop Plants*. John Wiley & Sons, Ltd, pp. 649–668.
- Ahmad, R., Waraich, E.A., Ashraf, M.Y., Ahmad, S., Aziz, T., 2014. Does nitrogen fertilization enhance drought tolerance in sunflower? A review. *J. Plant Nutr.* 37, 942–963.
- Ahmadi, M., Ascoug II, J.C., DeJonge, K.C., Arabi, M., 2014. Multisite-multivariable sensitivity analysis of distributed watershed models: enhancing the perceptions from computationally frugal methods. *Ecol. Model.* 279, 54–67.
- Ahuja, L.R., Reddy, V.R., Saseendran, S.A., Yu, Q. (Eds.), 2008. *Response of Crops to Limited Water: Understanding and Modeling Water Stress Effects on Plant Growth Processes*. ASA-CSSA-SSSA, Madison, Wisc.
- Ajami, N.K., Duan, Q.Y., Sorooshian, S., 2007. An integrated hydrologic Bayesian multimodel combination framework: confronting input, parameter, and model structural uncertainty in hydrologic prediction. *Water Resour. Res.* 43 (1), 19.
- Allen, R.G., Pereira, L.S., Raes, D., Smith, M., 1998. *Crop Evapotranspiration: Guidelines for Computing Crop Requirements*. FAO Irrigation and Drainage Paper No. 56, Rome, Italy.
- Arabi, M., 2011. *Environmental risk assessment and management system*. Colorado Water 28, 15–17.
- Baigorria, G.A., Jones, J.W., O'Brien, J.J., 2008. Potential predictability of crop yield using an ensemble climate forecast by a regional circulation model. *Agric. For. Meteorol.* 148, 1353–1361.
- Beven, K., Binley, A., 1992. The future of distributed models - model calibration and uncertainty prediction. *Hydrol. Process.* 6 (3), 279–298.
- Box, G.E.P., Cox, D.R., 1964. An analysis of transformations. *J. Roy. Stat. Soc. B Stat. Methodol.* 26 (2), 211–252.
- Box, G., Tiao, G., 1992. *Bayesian Inference in Statistical Analysis*. Wiley.
- Brumbelow, K., Georgakakos, A., 2007. Determining crop-water production functions using yield-irrigation gradient algorithms. *Agric. Water Manag.* 87 (2), 151–161.
- Ceglar, A., Crepinsek, Z., Kajfez-Bogataj, L., Pogacar, T., 2011. The simulation of phenological development in dynamic crop model the Bayesian comparison of different methods. *Agric. For. Meteorol.* 151 (1), 101–115.
- Chang, K.-H., Warland, J., Voroney, P., Bartlett, P., Wagner-Riddle, C., 2013. Using DayCent to simulate carbon dynamics in conventional and no-till agriculture. *Soil Sci. Soc. Am. J.* 77 (3), 941–950.
- Colorado Water Conservation Board, 2010. *Colorado's Water Supply Future. SWSI 2010 Mission Statement, Key Findings, and Recommendations*. State of Colorado.
- Confalonieri, R., et al., 2016. Uncertainty in crop model predictions: what is the role of users? *Environ. Model. Software* 81, 165–173.
- Corbeels, M., Chirat, G., Messad, S., Thierfelder, C., 2016. Performance and sensitivity of the DSSAT crop growth model in simulating maize yield under conservation agriculture. *Eur. J. Agron.* 76, 41–53.
- De Gryze, S., et al., 2010. Simulating greenhouse gas budgets of four California cropping systems under conventional and alternative management. *Ecol. Appl.* 20 (7), 1805–1819.
- DeJonge, K.C., Ascoug II, J.C., Ahmadi, M., Andales, A.A., Arabi, M., 2012. Global sensitivity and uncertainty analysis of a dynamic agroecosystem model under different irrigation treatments. *Ecol. Model.* 231, 113–125.

- Del Grosso, S.J., et al., 2006. DAYCENT national-scale simulations of nitrous oxide emissions from cropped soils in the United States. *J. Environ. Qual.* 35 (4), 1451–1460.
- Del Grosso, S.J., Halvorson, A.D., Parton, W.J., 2008. Testing DAYCENT model simulations of corn yields and nitrous oxide emissions in irrigated tillage systems in Colorado. *J. Environ. Qual.* 37 (4), 1383–1389.
- Del Grosso, S.J., Ogle, S.M., Parton, W.J., Breidt, F.J., 2010. Estimating uncertainty in N₂O emissions from US cropland soils. *Global Biogeochem. Cycles* 24.
- Doorenbos, J., Kassam, A., 1979. Yield response to water. *Irrigat. Drain. Pap.* 33, 257.
- Dozier, A.Q., Arabi, M., Wostoupal, B.C., Goemans, C.G., Zhang, Y., Paustian, K., 2017. Declining agricultural production in rapidly urbanizing semi-arid regions: policy tradeoffs and sustainability indicators. *Environ. Res. Lett.* 12, 085005.
- Dumont, B., et al., 2014. Parameter identification of the STICS crop model, using an accelerated formal MCMC approach. *Environ. Model. Software* 52, 121–135.
- Dzotsi, K.A., Basso, B., Jones, J.W., 2015. Parameter and uncertainty estimation for maize, peanut and cotton using the SALUS crop model. *Agric. Syst.* 135, 31–47.
- Eissa, M.A., Roshdy, N.M.K., 2019. Effect of nitrogen rates on drip irrigated maize grown under deficit irrigation. *J. Plant Nutr.* 42, 127–136.
- Engeland, K., Xu, C.-Y., Gottschalk, F., 2005. Assessing uncertainties in a conceptual water balance model using Bayesian methodology. *Hydrol. Sci. J.* 50, 45–63.
- English, M., 1990. Deficit irrigation. I: analytical framework. *J. Irrigat. Drain. Eng.* 116 (3), 399–412.
- Fereres, E., Soriano, M.A., 2007. Deficit irrigation for reducing agricultural water use. *J. Exp. Bot.* 58 (2), 147–159.
- Fitton, N., et al., 2014. Assessing the sensitivity of modelled estimates of N₂O emissions and yield to input uncertainty at a UK cropland experimental site using the DailyDayCent model. *Nutrient Cycl. Agroecosyst.* 99 (1–3), 119–133.
- Fragoso, T.M., Bertoli, W., Louzada, F., 2018. Bayesian model averaging: a systematic review and conceptual classification. *Int. Stat. Rev.* 86, 1–28.
- Garcia-Vila, M., Fereres, E., 2012. Combining the simulation crop model AquaCrop with an economic model for the optimization of irrigation management at farm level. *Eur. J. Agron.* 36 (1), 21–31.
- Gelman, A., Rubin, D.B., 1992. Inference from iterative simulation using multiple sequences. *Stat. Sci.* 7 (4), 457–472.
- Guillaume, J., Andrews, F., 2012. *Dream: Differential Evolution Adaptive Metropolis. R package version 0.4-2*. <http://CRAN.R-project.org/package=dream>.
- Haefner, J.W., 2005. *Modeling Biological Systems: Principles and Applications*. Springer Science & Business Media.
- He, J., Dukes, M.D., Jones, J.W., Graham, W.D., Judge, J., 2009. Applying glue for estimating CERES-Maize genetic and soil parameters for sweet corn production. *Transactions of the ASABE* 52 (6), 1907–1921.
- Iizumi, T., Tanaka, Y., Sakurai, G., Ishigooka, Y., Yokozawa, M., 2014. Dependency of parameter values of a crop model on the spatial scale of simulation. *J. Adv. Model. Earth Syst.* 6 (3), 527–540.
- Jarecki, M.K., Parkin, T.B., Chan, A.S.K., Hatfield, J.L., Jones, R., 2008. Comparison of DAYCENT-simulated and measured nitrous oxide emissions from a corn field. *J. Environ. Qual.* 37 (5), 1685–1690.
- Jha, P.K., Kumar, S.N., Ines, A.V.M., 2018. Responses of soybean to water stress and supplemental irrigation in upper Indo-Gangetic plain: field experiment and modeling approach. *Field Crop. Res.* 219, 76–86.
- Joint Research Center of the European Commission, 2004. *SIMLAB V2.2 - Simulation Environment for Uncertainty and Sensitivity Analysis*. European Commission - Institute for the Protection and Security of the Citizen.
- Laloy, E., Fasbender, D., Bielders, C.L., 2010. Parameter optimization and uncertainty analysis for plot-scale continuous modeling of runoff using a formal Bayesian approach. *J. Hydrol.* 380 (1–2), 82–93.
- Lee, J., De Gryze, S., Six, J., 2011. Effect of climate change on field crop production in California's Central Valley. *Climatic Change* 109, 335–353.
- Ma, L., Hoogenboom, G., Saseendran, S.A., Bartling, P.N.S., Ahuja, L.R., Green, T.R., 2009. Effects of estimating soil hydraulic properties and root growth factor on soil water balance and crop production. *Agron. J.* 101, 572–583.
- Marshall, L., Nott, D., Sharma, A., 2007. Towards dynamic catchment modelling: a Bayesian hierarchical mixtures of experts framework. *Hydrol. Process.* 21, 847–861.
- Maupin, M.A., Kenny, J.F., Hutson, S.S., L, J.K., B, N.L., Linsey, K.S., 2014. Estimated use of water in the United States in 2010: U.S. Geol. Surv. Circular 1405.
- McGuire, V.L., 2014. Water-level Changes and Change in Water in Storage in the High Plains Aquifer, Predevelopment to 2013 and 2011–13. U.S. Geological Survey Scientific Investigations. Report 2014-5218.
- Monsi, B., Saeki, T., 1953. Ueber den lichtfaktor in den pflanzengesellschaften und seine bedeutung für die stoffproduktion. *Jpn. J. Bot.* 14, 22–52.
- Necpalová, M., et al., 2015. Understanding the DayCent model: calibration, sensitivity, and identifiability through inverse modeling. *Environ. Model. Software* 66, 110–130.
- Parton, W.J., Hartman, M., Ojima, D., Schimel, D., 1998. DAYCENT and its land surface submodel: description and testing. *Global Planet. Change* 19 (1–4), 35–48.
- Parton, W.J., Schimel, D.S., Cole, C.V., Ojima, D.S., 1987. Analysis of factors controlling soil organic matter levels in great Plains grasslands 1. *Soil Sci. Soc. Am. J.* 51, 1173–1179.
- Pathak, T.B., Fraisse, C.W., Jones, J.W., Messina, C.D., Hoogenboom, G., 2007. Use of global sensitivity analysis for CROPGRO cotton model development. *Transactions of the ASABE* 50 (6), 2295–2302.
- Pathak, T.B., Jones, J.W., Fraisse, C.W., Wright, D., Hoogenboom, G., 2012. Uncertainty analysis and parameter estimation for the CSM-CROPGRO-Cotton model. *Agron. J.* 104 (5), 1363–1373.
- Paustian, K., Easter, M., Brown, K., Chambers, A., Eve, M., Huber, A., Marx, E., Layer, M., Stermer, M., Sutton, B., Swan, A., Toureene, C., Verlayudhan, S., Williams, S., 2018. Field- and farm-scale assessment of soil greenhouse gas mitigation using COMET-FarmTM, 2018. In: Delgado, J.A., Sassenrath, G.F., Mueller, T. (Eds.), *Precision Conservation: Geospatial Techniques for Agricultural and Natural Resources Conservation*. ASA/CSSA/SSSA, Madison WI, pp. 341–359. *Agronomy Monograph* 59.
- Saddique, Q., Cai, H., Ishaque, W., Chen, H., Chau, H.W., Chattha, M.U., Hassan, M.U., Khan, M.I., He, J., 2019. Optimizing the sowing date and irrigation strategy to improve maize yield by using CERES (crop estimation through Resource and environment synthesis)-maize model. *Agronomy* 9, 109.
- Saltelli, A., Chan, K., Scott, E.M., 2000. *Sensitivity Analysis: Gauging the Worth of Scientific Models*. Wiley.
- Saltelli, A., Ratto, M., Tarantola, S., Campolongo, F., 2005. Sensitivity analysis for chemical models. *Chem. Rev.* 105 (7), 2811–2827.
- Saltelli, A., Tarantola, S., Chan, K.P.S., 1999. A quantitative model-independent method for global sensitivity analysis of model output. *Technometrics* 41 (1), 39–56.
- Saseendran, S., Ahuja, L.R., Ma, L., Trout, T.J., McMaster, G.S., Nielsen, D.C., Ham, J.M., Andales, A.A., Halvorson, A.D., Chávez, J.L., 2014. Developing and normalizing average corn crop water production functions across years and locations using a system model. *Agric. Water Manag.* 157, 65–77.
- Saxton, K.E., Rawls, W.J., Romberger, J.S., Papendick, R.I., 1986. Estimating generalized soil-water characteristics from texture. *Soil Sci. Soc. Am. J.* 50 (4), 1031–1036.
- Sellers, P.J., 1985. Canopy reflectance, photosynthesis and transpiration. *Int. J. Rem. Sens.* 6 (8), 1335–1372.
- Sobol, I.M., 1993. Sensitivity estimates for nonlinear mathematical models. *Math. Model. Civ. Eng.* 1 (4), 407–414.
- Soltani, A., Sinclair, T.R., 2012. *Modeling Physiology of Crop Development, Growth and Yield*. CAB, Wallingford.
- Stedinger, J.R., Vogel, R.M., Lee, S.U., Batchelder, R., 2008. Appraisal of the generalized likelihood uncertainty estimation (GLUE) method. *Water Resour. Res.* 44.
- Stehfest, E., Heistermann, M., Priess, J.A., Ojima, D.S., Alcamo, J., 2007. Simulation of global crop production with the ecosystem model DayCent. *Ecol. Model.* 209 (2–4), 203–219.
- Sun, M., Zhang, X.L., Huo, Z.L., Feng, S.Y., Huang, G.H., Mao, X.M., 2016. Uncertainty and sensitivity assessments of an agricultural-hydrological model (RZWQM2) using the GLUE method. *J. Hydrol.* 534, 19–30.
- Suyker, A.E., Verma, S.B., 2009. Evapotranspiration of irrigated and rainfed maize-soybean cropping systems. *Agric. For. Meteorol.* 149 (3–4), 443–452.
- Trout, T.J., Bausch, W.C., Buchleiter, G., 2010. *Water Production Functions for Central Plains Crops*. 5th National Decennial Irrigation Conference Proceedings, Phoenix, AZ, pp. 5–8.
- Van Oijen, M., et al., 2011. A Bayesian framework for model calibration, comparison and analysis: application to four models for the biogeochemistry of a Norway spruce forest. *Agric. For. Meteorol.* 151 (12), 1609–1621.
- Varela, H., Guérif, M., Buis, S., 2010. Global sensitivity analysis measures the quality of parameter estimation: the case of soil parameters and a crop model. *Environ. Model. Software* 25 (3), 310–319.
- Verma, S.B., et al., 2005. Annual carbon dioxide exchange in irrigated and rainfed maize-based agroecosystems. *Agric. For. Meteorol.* 131 (1–2), 77–96.
- Vorosmarty, C.J., Green, P., Salisburry, J., Lammers, R.B., 2000. Global water resources: vulnerability from climate change and population growth. *Science* 289 (5477), 284–288.
- Vrugt, J.A., ter Braak, C.J.F., Clark, M.P., Hyman, J.M., Robinson, B.A., 2008. Treatment of input uncertainty in hydrologic modeling: doing hydrology backward with Markov chain Monte Carlo simulation. *Water Resour. Res.* 44.
- Vrugt, J.A., et al., 2009a. Accelerating Markov chain Monte Carlo simulation by differential evolution with self-adaptive randomized subspace sampling. *Int. J. Nonlinear Sci. Numer. Stimul.* 10 (3), 273–290.
- Vrugt, J.A., ter Braak, C.J.F., Gupta, H.V., Robinson, B.A., 2009b. Equifinality of formal (DREAM) and informal (GLUE) Bayesian approaches in hydrologic modeling? *Stoch. Environ. Res. Risk Assess.* 23 (7), 1011–1026.
- Vrugt, J.A., Ter Braak, C.J.F., 2011. DREAM((D)): an adaptive Markov chain Monte Carlo simulation algorithm to solve discrete, noncontinuous, and combinatorial posterior parameter estimation problems. *Hydrol. Earth Syst. Sci.* 15 (12), 3701–3713.
- Vrugt, J.A., 2016. Markov chain Monte Carlo simulation using the DREAM software package: theory, concepts, and MATLAB implementation. *Environ. Model. Software* 75, 273–316.
- Wang, X., He, X., Williams, J.R., Izaurralde, R.C., Atwood, J.D., 2005. Sensitivity and uncertainty analyses of crop yields and soil organic carbon simulated with EPIC. *Transactions of the ASAE* 48 (3), 1041–1054.
- Wang, G., Chen, S., 2012. A review on parameterization and uncertainty in modeling greenhouse gas emissions from soil. *Geoderma* 170, 206–216.
- Yin, X., Laar, H.H. van, 2005. *Crop Systems Dynamics: an Ecophysiological Simulation Model for Genotype-By-Environment Interactions*. Wageningen Academic Pub.
- Zhang, Y., Qian, Y.L., Bremer, D.J., Kaye, J.P., 2013. Simulation of nitrous oxide emissions and estimation of global warming potential in turfgrass systems using the DayCent Model. *J. Environ. Qual.* 42 (4), 1100–1108.
- Zhang, Y., 2016. *Simulating Canopy Dynamics, Productivity and Water Balance of Annual Crops from Field to Regional Scales*. PhD dissertation. Department of Soil and Crop Sciences. Colorado State University.
- Zhang, Y., Hansen, N., Trout, T., Nielson, D., Paustian, K., 2018a. Modeling deficit irrigation of maize with the DayCent model. *Agron. J.* 110, 1754–1764.
- Zhang, Y., Paustian, K., 2019. Sensitivity of predicted agro-ecosystem variables to errors in weather input data. *Transactions of the ASABE* 62, 627–640.
- Zhang, Y., Suyker, A., Paustian, K., 2018b. Improved crop canopy and water balance dynamics for agroecosystem modeling using DayCent. *Agron. J.* 110, 511–524.