Applying GLUE for Estimating CERES-Maize Genetic and Soil Parameters for Sweet Corn Production

J. He, M. D. Dukes, J. W. Jones, W. D. Graham, J. Judge

Abstract. *Sweet corn (*Zea mays *L.) is one of the five most valuable vegetable crops in Florida. The application of nitrogen fertilizer is necessary for farmers to reliably produce sweet corn. The use of crop simulation models can facilitate the evaluation of management practices that are profitable with minimal unwanted impacts on the environment. Before using such models in decision making, it is necessary to specify model parameters and understand the uncertainties associated with simulating variables that are needed for decision making. The generalized likelihood uncertainty estimation (GLUE) method was used to estimate genotype and soil parameters of the CERES-Maize model of the Decision Support System for Agrotechnology Transfer (DSSAT). The uncertainties in predictions for sweet corn production in northern Florida were evaluated using the existing field corn genotype coefficient and soil parameter database contained within DSSAT and field data collected during a series of experiments carried out in 2005 and 2006. Genotype coefficients (P1, P5, and PHINT) and soil parameters (SLDR, SLRO, SDUL, SLLL, and SSAT) were generated using a multivariate normal distribution that preserved the correlations between parameters. The soil parameter SLPF was not correlated with other parameters and was generated with a uniform distribution. After parameters were estimated, the CERES-Maize model correctly predicted the dry matter yields, anthesis dates, and harvest dates. The mean values of these variables were close to those measured in the field, with an average relative error of 4.4% and 2.4% for the data sets of 2005 and 2006, respectively. The calibrated CERES-Maize model simulated the temporal trend of leaf TKN concentration accurately during the early stage of the growth season, but underestimated the leaf TKN concentrations during the latter half of the season. The GLUE procedure accurately estimated soil parameters (SLLL, SDUL, and SSAT) when compared to independent measurements made in the laboratory, with an average absolute relative error of about 8.5%. The simulated time series of soil water content adequately simulated the observed soil water changes during both growth seasons for every layer. However, there were some large differences between simulated and observed soil nitrate contents. In a relevant further study, the average absolute relative error between model-predicted and field-estimated amounts of potential nitrogen leaching was 15.3%, which is much better than some reported comparable studies of nitrogen leaching modeling. In the posterior distribution of estimated parameters, the uncertainties in parameters were substantially reduced, with CV values mostly lower than 10%. The average CV value of the parameters was reduced from 27.2% in the prior distribution to 4.6% in the posterior distribution. In general, the results of this study showed that the CERES-Maize model was capable of simulating sweet corn production in northern Florida and the associated soil water content. The model can also simulate potential nitrogen leaching with acceptable accuracy. We suggest that the model can now be used to compare different management practices relative to productivity and potential nitrogen leaching outcomes.*

Keywords. *CERES-Maize, Crop model, DSSAT, Generalized likelihood uncertainty estimation, GLUE, Parameter estimation, Sweet corn.*

Sweet corn (*Zea mays* L.) has typically ranked as one of the five most valuable vegetable crops in Florida. During the 2000-2001 production seasons, sweet corn was the second ranked vegetable crop in terms of area planted and fifth in terms of total value in Florida (FASS, 2002). High amounts of nitrogen fertilizer are necessary for farmers to guarantee economic yields of sweet corn. Between 1992 and 2006, 81% to 100% of sweet corn acreage in Florida received an average of 2 to 10 applications of nitrogen (N) seasonally. An average range of 46 to 62 kg N ha^{-1} was used at each application, with a statewide annual total application amount of 1.64 to 5.48 million kg N (USDA-ERS, 1993; USDA-NASS, 1995, 1999, 2003, 2007).

Nitrogen leaching from sweet corn fields is economically and environmentally undesirable (Katyal et al., 1985; Poss and Saragoni, 1992; Theocharopoulos et al., 1993). Nitrate that leaches below the crop root zone represents the loss of a valuable plant nutrient, and hence an unnecessary cost. If nitrate enters groundwater supplies, it can also impose risks to both human health and the environment. Consumption of drinking water with high nitrate levels by human infants and young livestock has been associated with methemoglobinemia or blue baby syndrome. Additionally, groundwater with high nitrate levels that discharges into sensitive surface wa-

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ters can contribute to long-term eutrophication of those water bodies (Asadi et al., 2002). Thus, approaches have been proposed to protect water quality, such as the development of best management practices (BMPs) and grower education regarding sustainable fertilizer use in crop production (Florida, 1999).

Since it is expensive and time-consuming to test management practices through field experiments, the use of simulation models can facilitate the evaluation of different production practices and environments and thereby streamline the decision-making process (Rinaldi et al., 2007). Computer-based agronomic models are described as "quantitative schemes for predicting the growth, development, and yield of a crop, given a set of genotype coefficients and relevant environmental variables" (Monteith, 1996). The CERES-Maize model (Ritchie et al., 1998) imbedded in the Decision Support System of Agrotechnology Transfer (DSSAT) V 4.0 (Jones and Kiniry, 1986; Tsuji et al., 1994; Jones et al., 2003) is a well-known crop model developed for field corn production. This model simulates development and yield of different varieties of corn using genotype coefficients (Ritchie, 1998). Although this model has been used for a wide range of varieties or hybrids of field corn around the world (Wu et al., 1989; Steele et al., 1994; Gabrielle and Kengni, 1996; Pang et al., 1997a, 1997b, 1998; Jagtap et al., 1999; Asadi and Clemente, 2003), its utility for simulating sweet corn in Florida has not been demonstrated by currently available literature, and crop parameters were not specifically available for sweet corn in the DSSAT database. Thus, this study was undertaken to determine how well the CERES-Maize model could simulate sweet corn for use in evaluating management practices for production and environmental protection goals.

The application of crop models generally requires large amounts of data. The input data and model parameters are rarely known with certainty, since they can be difficult to determine accurately due to the inherent variability in natural processes, costly monitoring, or imperfections in data measurements (Wang et al., 2005). Proper estimation of model parameters is therefore required for ensuring accurate model predictions and good model-based decision rules (Makowski et al., 2002).

Traditional methods of parameter estimation have aimed at finding an optimal set of parameter values within some particular model structure (Mertens et al., 2004). The limitations of the optimal parameter set concept have been discussed by Beven and Binley (1992) and Beven (1993, 2001). They suggest that there is inherent uncertainty in parameters and that a number of parameter sets may be equally accepted in simulating the system. Given the observations available, there may be no rigorous basis for differentiating between these parameter sets. Beven (1993) introduced the term "equifinality" to address this problem. The most important implication of the equifinality problem is the non-uniqueness of the solution found by an inverse modeling or calibration process.

One response to the inherent uncertainty in parameters and the equifinality problem is to consider parameters as random variables and estimate their probability distributions instead of single values. One method that does this is the generalized likelihood uncertainty estimation (GLUE) approach (Mertens et al., 2004), a Bayesian Monte Carlo technique (Candela et al., 2005) that uses observed data and prior information about parameter distributions. A first step in the GLUE approach is to define a prior parameter probability distribution based on literature or expert knowledge. The prior distribution can be, for example, a uniform distribution with lower and upper bounds derived from expert knowledge or a normal distribution. The second step consists of calculating a posterior probability distribution from both the prior distribution and available data, such as observed crop yields, soil moisture, and biomass nutrient concentration. This posterior distribution, computed using Bayes theorem, is used to estimate the most likely parameter set and the uncertainties of parameters and model outputs (Makowski et al., 2006).

The objectives of this study were to estimate the genetic coefficients and soil parameters of the CERES-Maize model in DSSAT with the GLUE method and to assess the uncertainties in the use of this model for simulating the growth (including phenology dates, dry matter yield, etc.) and nitrogen leaching of sweet corn production in northern Florida.

Materials and Methods

CERES-Maize Model

Crop growth and development are simulated by the CERES-Maize model (V 4.0; Hoogenboom et al., 2003) with a daily time step from planting to maturity based on physiological processes that describe the responses of maize to soil and environmental conditions. Potential growth is dependent on photosynthetically active radiation and its interception, whereas actual biomass production on any day is constrained by suboptimal temperatures, soil water deficits, and nitrogen deficiencies (Ritchie and Godwin, 1989; Ritchie, 1998). Since CERES-Maize V4.0 does not directly simulate ear fresh weight, which is the product harvest in sweet corn production, the question may arise whether it can be inferred from grain dry weight that ear fresh weight at sweet corn harvest can be simulated adequately. Lizaso et al. (2007) published a model of sweet corn growth and yield based on the CERES-Maize model. The version of CERES-Maize that they modified to create the new model was also CERES-Maize V4.0. This new model simulates the increase in ear dry weight concentration (DMC), expressed as a fraction of ear fresh weight, with a slope of 0.0002 per unit of thermal time. Fresh weight of ears (FW_{ear} , g plant^{-1}) is calculated as (Lizaso et al., 2007):

$$FW_{ear} = \frac{DW_{ear}}{DMC} \tag{1}$$

where DW_{ear} is the ear dry weight (g plant^{-1}). Using the plant population density and FW_{ear}, the model calculates total fresh weight yield of ears (TotFW, kg ha^{-1}). Thus, if the value of DMC and DW_{ear} were known, the value of FW_{ear} could be simply calculated through this equation. The work of Lizaso et al. (2007), which was done somewhat in parallel with this study, did a very good job of simulating sweet corn production in northern Florida. In this study, it was found the DMC value at harvest of the sweet corn variety used was very stable at about 15%. Thus, this equation was used to bridge the gap between fresh ear yield and dry ear yield.

Generally, there are four types of input data to the CERES-Maize model: weather, crop, soil, and management. The weather inputs are the daily sum of global radiation (MJ m^{-2}), the daily minimum and maximum air temperatures (°C), and the daily sum of precipitation (mm) (Ritchie, 1998). In this

Table 1. Soil parameters for the CERES-Maize model in DSSAT.

Parameter	Definition	Type	Mean	Unit
SLLL	Lower limit for plant uptake	Layered	0.13	m^3 m^{-3}
SDUL	Drained upper limit	Layered	0.25	m^3 m^{-3}
SSAT	Soil saturation water content	Layered	0.38	m^3 m^{-3}
SBDM	Soil bulk density	Layered	1.32	g cm^{-3}
SALB	Soil albedo	Single	0.13	--
SLU1	Soil evaporation limit	Single	6	mm
SLRO	Soil runoff curve number	Single	73	--
SLDR	Soil drainage rate	Single	0.46	fraction d^{-1}
SLPF	Growth reduction/fertility factor that accounts for the effects of soil nutrients (other than nitrogen) on daily plant growth rate.	Single	0.96	--

Table 2. Genotype coefficients for the CERES-Maize model in DSSAT.

Parameter	Definition	Mean	Unit
P1	Thermal time from seedling emergence to the end of the juvenile phase (expressed in degree days above 8°C base temperature) during which the plant is not responsive to changes in photoperiod.	225	degree days
P2	Extent to which development is delayed (in days) for each hour increase in photoperiod above the longest photoperiod at which development proceeds at maximum rate (which is considered to be 12.5 h).	0.52	--
P5	Thermal time from silking to harvest maturity (expressed in degree days above 8°C base temperature).	764	degree days
G2	Maximum possible number of kernels per plant.	811	--
G3	Kernel filling rate during the linear grain filling stage and under optimum conditions.	8.5	mg day^{-1}
PHINT	Phylochron interval; the interval in thermal time (degree days) between successive leaf tip appearances.	41.2	degree days

study, these data were directly obtained from the historical records from the Florida Automated Weather Network (FAWN; http://fawn.ifas.ufl.edu/) at the experiment site: the Plant Science Research and Education Unit (29.4094° N, 82.1777° W, 21 m above sea level) at the University of Florida. Required crop management information including planting density, row spacing, planting depth, irrigation dates and amounts, and application of N fertilizer (Ritchie, 1998) were also obtained from the field experiment. Crop physiological parameters are given in the form of genotype coefficients, which describe physiological processes such as development and growth for individual crop varieties. Soil parameters describe the physical, chemical, and morphological properties of the soil layers. Prior distributions of both field corn genotype coefficients and soil parameters needed for the GLUE procedure were taken from the DSSAT database, which contains coefficient values for a wide range of field corn varieties and soils ranging from sand to clay.

Soil Parameters and Genotype Coefficients

The layered soil parameters SLLL, SDUL, and SSAT (table 1) influence the amount of available water in the soil profile. The single soil parameters SLU1, SLRO, and SLDP influence the amount of water that infiltrates, evaporates, or drains from the soil profile, respectively. Parameter SLPF represents the effect of micronutrients or other unknown soil constraints on crop growth rates. Genotype coefficients P1, P2, and P5 (table 2) control the important phenology events, such as anthesis and harvest dates of corn. Coefficients G2 and G3 control the yield-related outputs, such as dry matter yield, canopy weight, etc., whereas coefficient PHINT influences both phenology dates and yield (Kiniry, 1991; Kiniry and Bonhomme, 1991). In these tables, the mean values of the parameters that were derived from DSSAT database are also listed.

Field Experiment

In this study, observations were obtained from the fourth and fifth Microwave, Water, and Energy Balance Experiments, MicroWEX-4 and -5 (Casanova et al., 2007; Casanova et al., 2006). The experiments were conducted on a 3.65 ha field site at the Plant Science Research and Education Unit, the University of Florida, located near Citra, Florida.

Sweet corn of variety ‘Saturn SH2’ was planted during each of two experimental years on 9 March 2005 and 9 March 2006 at a depth of 3.8 cm and a planting population density of 59,000 plants ha^{-1}. The harvest dates were 2 June 2005 and 1 June 2006, during MicroWEX-4 and -5, respectively. The nitrogen fertilizer used in the experiment was a composite of several nitrogen compounds (7.9% nitrate nitrogen, 7.9% ammoniacal nitrogen, and 16.2% urea nitrogen) and was applied weekly by injection through the linear-move sprinkler irrigation system (fertigation) beginning at four weeks after planting and ending one week before harvest. Liquid N fertilizer was applied at planting at a rate of 15 kg N ha^{-1}. There were seven fertigation events in the entire season for both experiments, with each event including 60 kg N ha^{-1} for a total of 422 kg N ha^{-1} over the season. Other agronomic practices, such as potassium fertilizer, herbicide, and pesticide application followed the recommendations of the Institute of Food and Agricultural Science, University of Florida (Olson and Simonne, 2005). Daily reference evapotranspiration (ET_0) and precipitation were obtained from the FAWN at the Citra measurement station and were used to schedule the timing and depth of irrigation events to maintain the soil water balance above the maximum allowable depletion, which was 50% of the calculated available water holding capacity.

The soil in the field was coarse and mapped as Lake Sand, Candler Variant, Tavares Variant, and Millhopper Variant 1, which mainly belong to Quartzipsamments (Entisol). To measure soil water holding characteristics, soil samples were collected from 24 locations at three depths (0-15 cm, 15-30 cm, and 30-60 cm) throughout the field. The samples were analyzed in the Department of Soil and Water Science, University of Florida. The intact soil core method was used to measure the values of permanent wilting point (SLLL) and field capacity (SDUL) (Klute, 1986). Soil bulk density was also measured. The SLLL was taken as the soil moisture at a soil pressure of 1.53 MPa, SDUL as the soil moisture at 0.01 MPa, and soil saturation (SSAT) as the soil moisture at 0 MPa (Ratliff et al., 1983). In this study, these independently measured soil properties were compared with the estimated soil parameter values as one way to evaluate the reliability of the parameter estimation procedure.

During the MicroWEX field experiments, biweekly soil samples were collected in the growth season to measure gravimetric soil water contents, and KCL extractable soil nitrate and ammonium concentrations using the colorimetric method (Page et al., 1982). The gravimetric soil moisture content was converted to volumetric soil moisture content with the measured soil bulk density. Samples were collected with an auger at each of eight sampling locations at four depths (0-15 cm, 15-30 cm, 30-60 cm, and 60-90 cm) in the field. The samples were analyzed in the Department of Soil and Water Science, University of Florida.

Biweekly crop leaf samples were collected at eight locations that were near the soil sampling points. For each sample, an entire plant that had an average height and size in the sampling area was collected. The samples were stored on ice and then processed in the lab. Total Kjeldahl nitrogen (TKN) of leaf tissue (including both green and senesced leaf tissue) was measured. The leaf samples were dried in an oven at a constant temperature of 60°C for 48 h. The dry samples were processed using the Kjeldahl procedure (Page et al., 1982) to determine TKN concentration in the Analytical Research Laboratory (ARL), Institute of Food and Agricultural Sciences, University of Florida.

Fresh ear yield (including husks and cob) was measured when the sweet corn reached fresh market maturity, about 70 to 80 days after planting. All corn ears in a sampling zone, which consisted of a 6.1 m section of two rows near each of eight sampling locations, were collected whether the kernels were fully filled or not. Then the ear samples were also dried in an oven at a constant temperature of 60°C for 48 h. Dry matter yield was calculated according to the measured fresh ear yield and average ear moisture. The dates and methods of planting, tillage, irrigation, fertigation, pesticide and herbicide application, and harvest were recorded. Critical dates for sweet corn development, such as tasseling, silking, and harvest maturity, were also recorded through direct *in situ* observations. Attention should be paid to definition of harvest date in this study. Unlike field corn varieties, which are harvested when the kernels are dry and fully mature (dent stage), sweet corn is picked when it is immature (milk stage) and eaten as a vegetable, rather than a grain. Thus, the maturity date here is the harvest date, rather than the physiological maturity date. Consequently, in the model, parameter P5 was defined as the thermal time from silking to harvest, as shown in table 2. The harvest date is measured by growers by watching the ear development. Typically about 14 to 18 days are required from pollination to edible ears, and silks will turn brown at that time.

GLUE Implementation

The main steps of the GLUE procedure used in this study were based on Beven and Binley (1992) and are summarized as follows:

Step 1. Select the soil parameters and genotype coefficients to be estimated with the GLUE method. A sensitivity analysis was previously performed with the non-interactive and interactive one-at-a-time (OAT) method (Morris, 1991) to determine which parameters to estimate (He, 2008). This analysis indicated that only the genotype and soil parameters shown in table 3 significantly influenced the model outputs of interest. These were dry matter yield (kg ha^{-1}) and cumulative nitrogen leaching (kg ha^{-1}), which are the two main outputs of concern for future studies on best management practices for sweet corn production. Although the values of soil parameters SLLL, SDUL, and SSAT were measured in independent field experiments, as mentioned before, they were also involved in the estimation procedure. This was done to demonstrate that the GLUE procedure could estimate these parameters starting with a wide range of data (all soils from the DSSAT database) in the absence of field measurements. Hence, the comparisons between actually measured and GLUE-estimated soil parameter values will be useful to determine the accuracy of the GLUE method. The other soil parameters in table 3 have to be estimated because they are difficult to measure or are empirical values. The parameters that were not selected for estimation were fixed at their mean values derived from the DSSAT database (as shown in tables 1 and 2).

Step 2. Estimate the probability distribution functions, means, and covariance of the parameters included in table 3 from the DSSAT V 4.0 database (Hoogenboom et al., 2003). A Jarque-Bera normality test (Judge et al., 1982) was conducted to determine whether these parameters followed normal distributions. Results showed that most corn genotype coefficients and soil parameters contained within the DSSAT database were normally distributed at a significance level of 90%. The crop genetic coefficients were correlated with each other, and the soil parameters were correlated with each other. It was anticipated that there was no correlation between genetic coefficients and soil parameters. There were strong correlations between soil parameters SLLL, SDUL, and SSAT. For example, the correlation coefficient was 0.94 between SLLL and SDUL, 0.58 between SLLL and SSAT, and 0.65 between SDUL and SSAT. Thus, in this study, except for SLPF, a multivariate normal distribution was accepted and used as the prior distribution for the selected input parameters. A uniform distribution of [0.7, 1.0] was assigned for SLPF, where 0.7 and 1.0 were the minimum and maximum, respectively, of SLPF in the DSSAT database. The covariance matrix of the selected parameters calculated from the DSSAT database (except for SLPF) is shown in table 4, which presents the correlations among the selected input parame-

Table 3. Selected parameters and their mean values for the GLUE method based on sensitivity analysis of predicted dry yield and cumulative nitrogen leaching (from He, 2008).

Parameter	P1 (°Cd)[a]	P5 (°Cd)	PHINT (°Cd)	SLDR (fraction d^{-1})	SLRO (--)	SLLL (cm^3 cm^{-3})	SDUL (cm^3 cm^{-3})	SSAT cm^3 cm^{-3})	SLPF (--)
Mean	225	764	41	0.46	73	0.13	0.25	0.38	0.96

[a] °Cd = degree day.

Table 4. Covariance matrix of the prior distribution.

	P1	P5	PHINT	SLDR	SLRO	SDUL	SLLL	SSAT
P1	4562	2374	62	0	0	0	0	0
P5	2374	9679	56	0	0	0	0	0
PHINT	62	56	16	0	0	0	0	0
SLDR	0	0	0	0.036	-0.339	-0.003	-0.003	-0.005
SLRO	0	0	0	-0.339	132	0.314	0.236	0.259
SDUL	0	0	0	-0.003	0.314	0.010	0.008	0.006
SLLL	0	0	0	-0.003	0.236	0.008	0.007	0.005
SSAT	0	0	0	-0.005	0.259	0.006	0.005	0.009

ters and will be used as the prior distribution to generate random parameter values later.

Step 3. Generate 10,000 random parameter sets from the prior distribution described in step 2. In this study, a Matlab (2004) program (mvnrnd.m) was used to generate random parameter sets. The function MVNRND (MU, SIGMA, CASES) returns a matrix of random numbers chosen from the multivariate normal distribution with mean vector MU (table 3) and covariance matrix SIGMA (table 4). CASES is the number of rows in the matrix, or the number of random parameter sets. The soil profile was divided into four layers: 0-15 cm, 15-30 cm, 30-60 cm, and 60-90 cm. For the layered parameters, such as SLLL, SDUL, and SSAT, values were assigned for each layer by assuming perfect correlation among the soil layers. In this way, only one random number is required to be generated for the first layer, while the values of other layers can be calculated through their correlation. For each generated random number for a layer 1 parameter, perturbations for the parameters in lower layers were calculated as follows:

$$\varepsilon_i = \frac{x1_i - \mu 1}{\sigma 1} \tag{2}$$

where ε_i is the perturbation, $x1_i$ is the ith generated normally distributed random sample for a soil property for layer 1, and $\mu 1$ and $\sigma 1$ are the mean and standard deviation, respectively, of the soil property of layer 1. For the soil property of layer 2, the ith random number, $x2_i$ was calculated as:

$$x2_i = \mu 2 + \varepsilon_i \cdot \sigma 2 \tag{3}$$

where $\mu 2$ is the mean and $\sigma 2$ is the standard deviation of the soil property of layer 2. The same approach was used to calculate the input values for all layers.

Step 4. Run the CERES-Maize model with the 10,000 generated random parameter sets. The model runs were implemented with Matlab in this study. The soil input file (soil.sol) and genotype input file for maize (MZCER040.cul) were replaced with a different set of generated random parameter values for each run. The outputs (dry yield, anthesis date, maturity date, leaf TKN content, soil nitrate concentration, and soil volumetric moisture) were saved after each simulation.

Step 5. Calculate the likelihood values $L(\theta_i|Y)$ for the different generated parameter vectors θ_i conditioned with observation Y using the selected likelihood function. The likelihood values derived from different types of observations were then combined (for details on this procedure, see the Likelihood Function section below).

Step 6. Calculate the probability p_i of the ith parameter set with following equation:

$$p(\theta_i) = \frac{L(\theta_i \mid Y)}{\sum_{j=1}^{N} L(\theta_i \mid Y)} \tag{4}$$

where $p(\theta_i)$ is the probability or likelihood weight of the ith parameter set θ_i, and $L(\theta_i|Y)$ is the likelihood value of parameter set θ_i.

Step 7. Use the pairs of parameter set and probability, (θ_i, p_i), $I = 1, ..., N$, to construct the posterior distribution and compute mean and variance of the posterior parameters with the following equations:

$$\hat{\mu}_{post}(\theta) = \sum_{i=1}^{N} p(\theta_i) \cdot \theta_i \tag{5}$$

$$\hat{\sigma}^2_{post}(\theta) = \sum_{i=1}^{N} p(\theta_i) \cdot (\theta_i - \hat{\mu}_{post})^2 \tag{6}$$

where $\hat{\mu}_{post}(\theta)$ and $\hat{\sigma}^2_{post}(\theta)$ are the estimated mean value and variance of the posterior distribution of parameters θ, $p(\theta_i)$ is the probability of the ith parameter set θ_i, $p(\theta_i)$ is the probability calculated by equation 4, and N is the number of random parameter sets.

Step 8. Compare the simulated and measured model output variables and soil parameters to evaluate the ability of the CERES-Maize model to correctly predict parameters and model states after the GLUE procedure. The absolute relative error (ARE) between simulated and measured variables was calculated for each pair of variables with equation 7 because this measure can be used for comparing errors based on different data sets and it is independent of the units of simulated and measured variables:

$$\text{ARE} = \frac{\left|Y - \hat{Y}\right|}{\hat{Y}} \times 100\% \tag{7}$$

where Y and $\hat{Y}$ are simulated and measured variable, respectively.

Likelihood Function

A likelihood function is required to calculate the likelihood value that measures the goodness-of-fit in comparing observations and predictions of the model with different random parameter sets. A method is also needed to combine the likelihood values derived from observations with different units. According to He (2008), the likelihood function and method of likelihood combination can heavily influence the

Table 5. Simulated and measured yields, anthesis dates, harvest dates in 2005 and 2006.

		Simulation				Measurement		
		Mean	SD	CV (%)	ARE (%)	Mean	SD	CV (%)
2005	Yield (kg ha^{-1})	2719	383	14	5.5	2878	269	9
	Anthesis date (days)	53	1.3	2	3.6	51	3.4	7
	Harvest date (days)	85	1.3	2	4.2	82	2.4	3
	Average	--	--	--	4.4	--	--	--
2006	Yield (kg ha^{-1})	3142	485	15	2.0	3206	121	4
	Anthesis date (days)	51	2.4	5	0.8	51	2.2	4
	Maturity date (days)	85	2.5	3	4.3	81	3.7	5
	Average	--	--	--	2.4	--	--	--

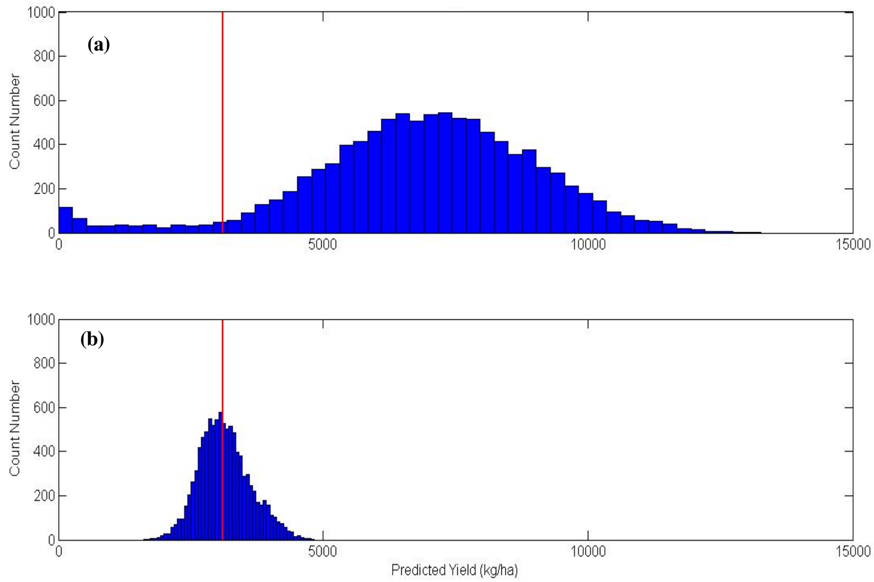

Figure 1. Histogram of predicted dry matter grain yield in 2006 under (a) prior and (b) posterior distributions. Vertical line represents average field-measured dry yield.

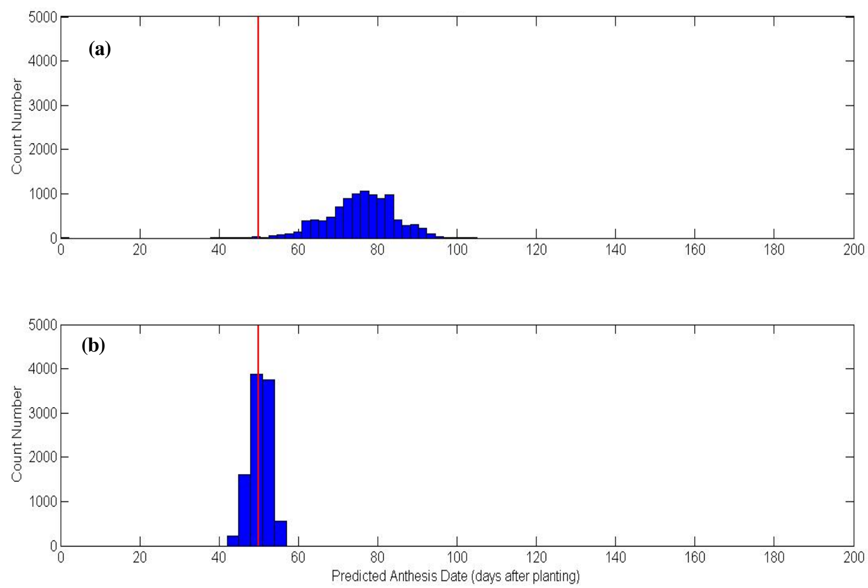

Figure 2. Histogram of predicted anthesis dates in 2006 under (a) prior and (b) posterior distributions. Vertical line represents average field-measured anthesis date.

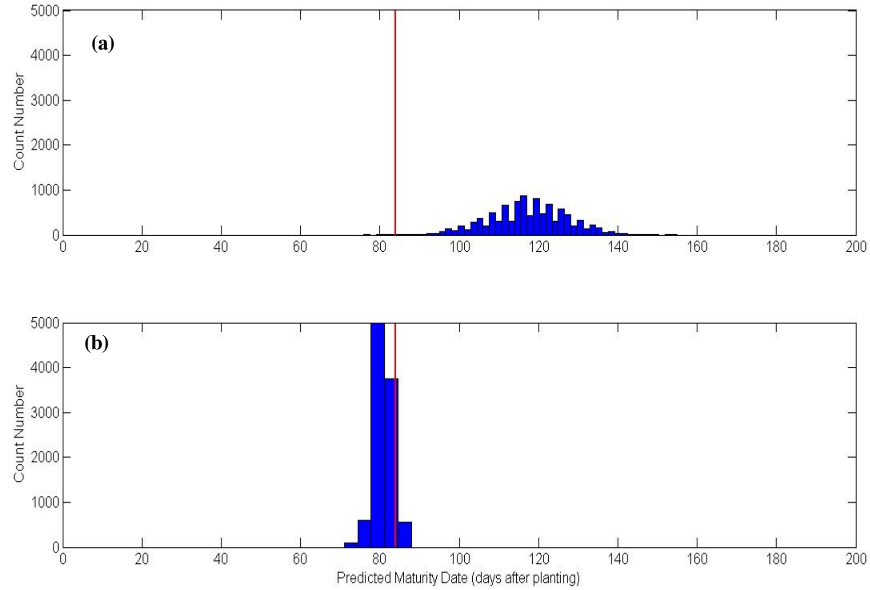

Figure 3. Histogram of predicted harvest maturity dates in 2006 under (a) prior and (b) posterior distributions. Vertical line represents average field-measured maturity date.

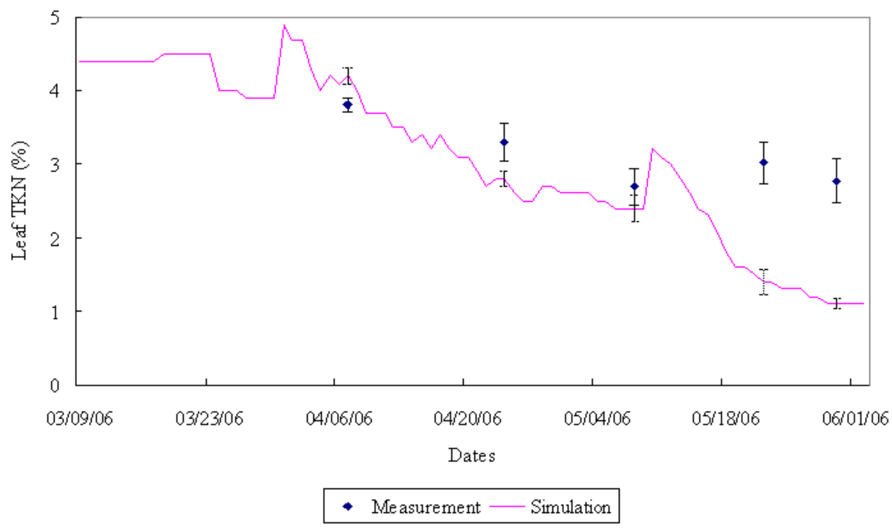

Figure 4. Measured and simulated leaf TKN concentrations over the sweet corn season in 2006. Error bars are standard deviations of measurements and simulations.

results of the GLUE procedure. Stedinger et al. (2008) criticized the use of an arbitrary likelihood function in GLUE. The choice of a likelihood function is critical, and the function needs to be a reasonable description of the distribution of the model errors for the statistical inference and resulting uncertainty and prediction intervals to be valid. He et al. (2009) found that the Gaussian likelihood function below (see Makowski et al., 2006) was successful in estimating parameters for CERES-Maize in a synthetic experiment study and recommended its use over other functions:

$$L[\theta_i \mid O] = \prod_{j=1}^{M} \frac{1}{\sqrt{2\pi\sigma_o^2}} \exp\left(-\frac{\left(O_j - Y(\theta_i)\right)^2}{2\sigma_o^2}\right) \quad (8)$$

$$(i = 1, 2, 3, \ldots, N)$$

where θ_i is the ith parameter set, $Y(\theta_i)$ is the model output using parameter set θ_i, O is the observation, O_j is the jth replicate of O, σ_o^2 is the variance of observations, and M is the number of observation replicates. In this study, equation 8 was used as the likelihood function for each observation type (dry matter yield, anthesis date, harvest date, leaf TKN concentration, soil nitrate concentration, and soil volumetric water content).

Dry matter yield, anthesis date (ADAT), and harvest date (HDAT) were integrated observations, which means there was only one observation value for each of them in the entire growth season. Leaf TKN concentration was a temporally variant observation. Soil nitrate concentration and volumetric moisture content were both temporally and spatially variable. Based on an analysis by He et al. (2009), a Bayesian multiplication method (eq. 9, from Beven and Binley, 1992)

Table 6. Measured and estimated mean values of soil properties of the field experiment site where DSSAT parameters SLLL, SDUL, and SSAT are permanent wilting point, field capacity, and saturated water content, respectively.

	SLLL (cm^3 cm^{-3})			SDUL (cm^3 cm^{-3})			SSAT (cm^3 cm^{-3})		
	Measured	Estimated	ARE	Measured	Estimated	ARE	Measured	Estimated	ARE
Mean	0.051	0.060	15.0%	0.110	0.104	5.8%	0.314	0.300	4.7%
SD	0.031	0.002	--	0.044	0.002	--	0.07	0.021	--
CV	61%	3%	--	40%	2%	--	22%	7%	--

Figure 5. Measured and simulated soil moisture at 0-15 cm over the sweet corn season in 2006. Error bars are standard deviations of measurements and simulations.

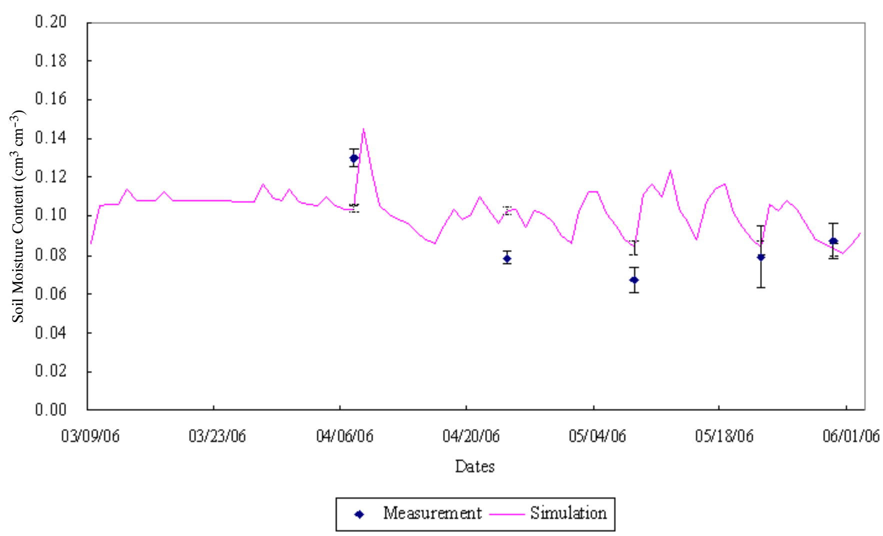

Figure 6. Measured and simulated soil moisture at 15-30 cm over the sweet corn season in 2006. Error bars are standard deviations of measurements and simulations.

was selected to combine likelihood values computed for different type of observations. This method efficiently eliminates the parameter sets that simultaneously give good predictions for some observations and poor predictions for other observations (He et al., 2009):

$$L_{combined} = \prod_{k=1}^{K} L_k [\theta_i | O] \tag{9}$$

where $L_{combined}$ is the combined likelihood value, $L_k[\theta_i|O]$ indicates the likelihood value of the kth type of observation conditioned with the ith parameter set θ_i and observation O, and K is the number of observation types.

A two-step GLUE procedure was conducted with the input variables (weather and field management) and observation data of the field experiment in 2005 and 2006. In the first step of GLUE, the first posterior distribution of parameters was derived from the calculated N pairs (θ_i, $p_i|i$ = 1, ..., N), where θ_i is the ith parameter set, and p_i is the calculated probability of the ith parameter set, conditioned on the observations O obtained in 2005. Then this first posterior distribution was used as the new prior distribution for the second step of

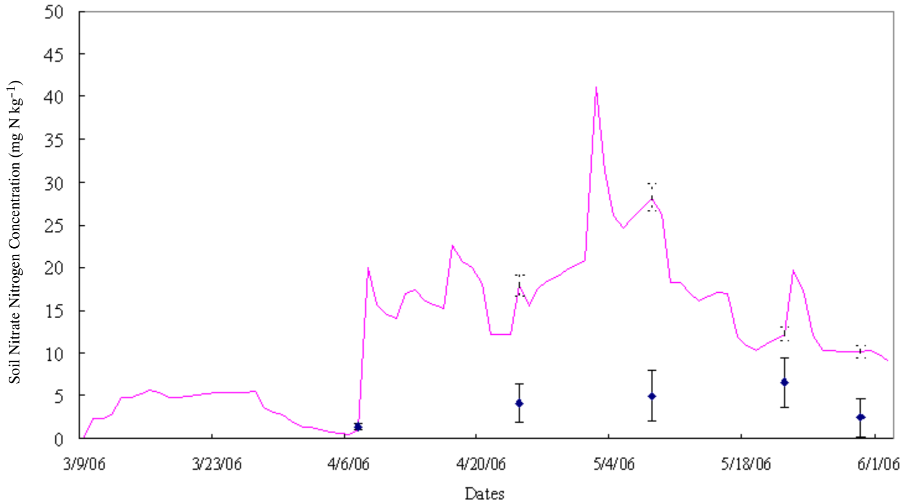

Figure 7. Measured and simulated soil nitrate content at 0-15 cm over the sweet corn season in 2006. Error bars are standard deviations of measurements and simulations.

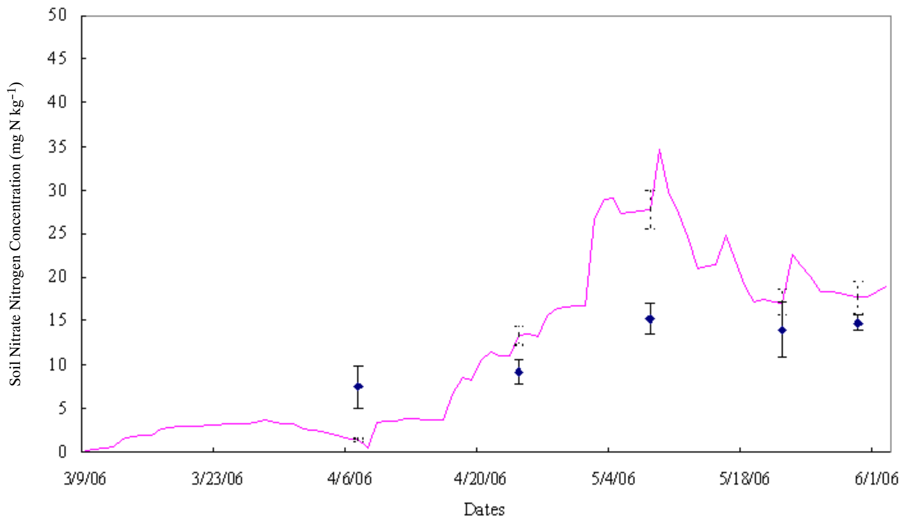

Figure 8. Measured and simulated soil nitrate content at 15-30 cm over the sweet corn season in 2006. Error bars are standard deviations of measurements and simulations.

GLUE that used the 2006 observations to create a final posterior distribution for subsequent analyses.

Results and Discussion

Comparison of Simulated and Observed Crop Variables

In general, the CERES-Maize model predicted crop variables in good agreement with observations using the soil and genotype parameters estimated after two rounds of GLUE (table 5). The calculated average absolute relative error (ARE) value between mean values of simulated and measured crop growth variables was 4.4% and 2.4% for the data sets of 2005 and 2006, respectively. In 2005, the predicted standard deviations of 383 kg ha^{-1}, 1.3 days, and 1.3 days after planting were 14%, 2%, and 2% of mean values of dry matter yield, anthesis, and harvest date. In 2006, the CV values of these output variables were 15%, 5%, and 3%, respectively.

As shown in the prior and posterior distributions of predicted yields, anthesis, and harvest dates (figs. 1 through 3), prediction uncertainties in these variable were significantly reduced after application of the GLUE procedure with the data of 2005 and 2006. For brevity, only the 2006 data are presented, but the trends of these variables were similar in 2005.

Measurements of leaf TKN taken five times in the growing season were compared with simulated values after estimating soil and crop parameters (fig. 4). In figure 4, the parameter set that had the maximum likelihood value was used to simulate the daily results shown by the solid line. Standard deviations of the simulations based on the entire posterior distribution of parameters are also shown by error bars. The mean values of TKN measurements and associated measurement standard deviations are also shown on this figure. During the early stage of the growth season, the calibrated CERES-Maize model simulated the temporal trend of leaf TKN concentration accurately, since the errors between predictions and observations were not significant. However, the calibrated model underestimated the leaf TKN concentrations during the latter half of the season. The last two mea-

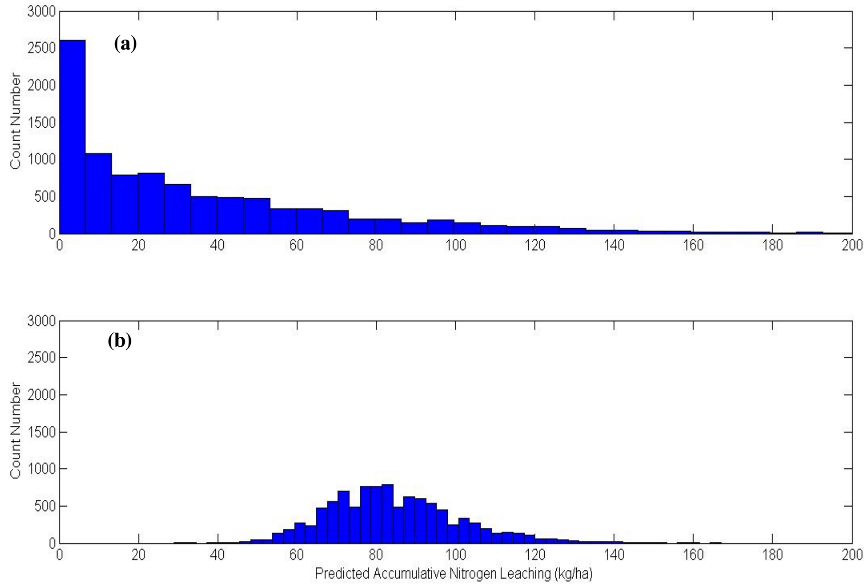

Figure 9. Histogram of predicted nitrate nitrogen leaching in 2006 under (a) prior and (b) posterior distributions.

Table 7. Fundamental statistical properties of prior and posterior distributions.

	Min.	Max.	Mean	SD	CV
Prior Distribution					
P1	110	450	225	68	30%
P5	580	1000	764	99	13%
PHINT	30	50	41	4	10%
SLDR	0.00	1.00	0.46	0.19	41%
SLRO	30	95	73	12	16%
SDUL	0.09	0.47	0.26	0.10	38%
SLLL	0.02	0.35	0.14	0.08	61%
SSAT	0.23	0.70	0.39	0.09	24%
SLPF	0.70	1.00	0.96	0.11	12%
Average	--	--	--	--	27%
Posterior Distribution					
P1	78	182	99	8	8%
P5	553	676	577	10	2%
PHINT	39	42	40	0.20	1%
SLDR	0.71	0.75	0.73	0.006	1%
SLRO	41	100	78	10	12%
SDUL	0.10	0.11	0.10	0.002	2%
SLLL	0.05	0.07	0.06	0.002	4%
SSAT	0.24	0.36	0.30	0.02	7%
SLPF	0.76	0.93	0.87	0.04	5%
Average	--	--	--	--	5%

sured mean values of leaf TKN were 3.02% and 2.78%, while the simulated mean values were only 1.4% and 1.1%. Two reasons might contribute to the difference between model predictions and field observations. First, the CERES-Maize model simulates the amount of N in stover, and the N is then portioned into leaves and stems according to the dry matter mass of each tissue. This results in identical N concentration in leaves and stems, which usually means underestimating N in leaves and the contrary in stems. In addition, fertigation events until late in the season may have maintained high leaf N content.

Comparison of Simulated and Observed Soil Variables

The GLUE-estimated soil parameters were close to the independently measured values (table 6). For example, the mean value of estimated SDUL in the posterior distribution was 0.104 $cm^3\ cm^{-3}$, while the mean measured SDUL was 0.110 $cm^3\ cm^{-3}$, with an ARE of 5.8%. The average ARE value for all soil water holding parameters was about 8.5%. This result suggests that the parameters that influence soil water holding capacity were all accurately estimated with the GLUE procedure, even though the prior distribution contained parameter values for soils that ranged from sand to clay. Volumetric soil water content measured on five dates was used in the parameter estimation process. Simulated and measured soil water of the two top soil layers (0-15 and 15-30 cm) were in good agreement (figs. 5 and 6). Data from deeper layers (i.e., 30-60 cm and 60-90 cm) are not shown, but the results were similar. However, there were substantial differences between simulated and observed soil nitrate contents of the two top soil layers (0-15 and 15-30 cm) (figs. 7 and 8). Especially for the 0-15 cm layer, except for the first one, measurements were all lower than the predictions in this layer. Unlike soil moisture, nitrate is very unstable in soil. It is difficult to accurately measure the soil nitrate content under the experimental conditions of this study. The complexity and difficulty in the simulation of soil nitrogen dynamics might also contribute to the discrepancy. Thus, future improvements should be made to the soil N simulation module. The mean value and standard deviation of the posterior distribution of simulated amounts of potential nitrate nitrogen leaching were 84.5 and 16.7 kg N ha^{-1}, while they were 39.0 and 46.8 kg N ha^{-1} under the prior distribution (fig. 9). The data of 2005 was not presented here, but the trend of this output variable was similar.

Although the uncertainty in this variable was also significantly reduced, we could not conclude that the model can correctly predict the amount of nitrogen leaching in the production system of sweet corn, since there was no direct

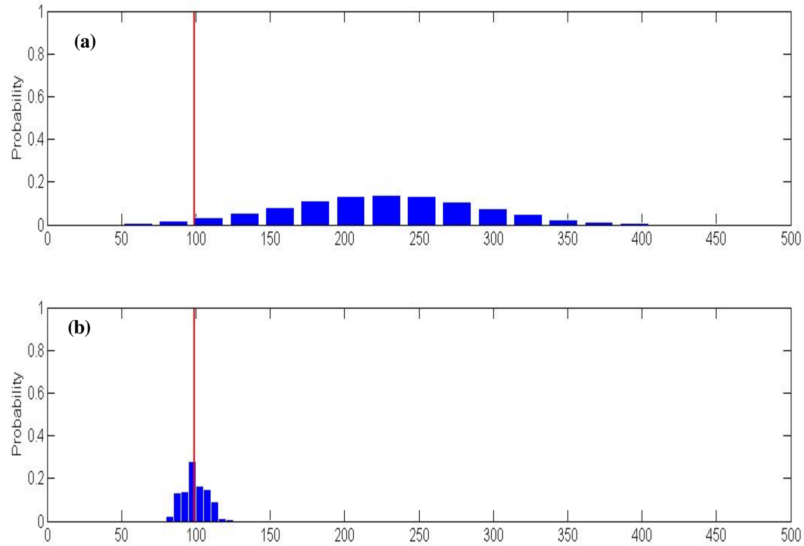

Figure 10. Parameter P1: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

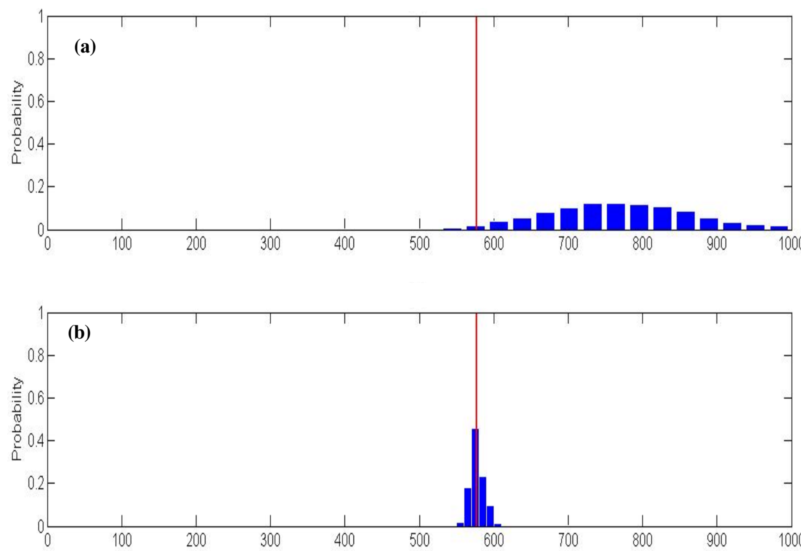

Figure 11. Parameter P5: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

field measurement for this variable in this study. However, He (2008) compared the model-predicted and field-estimated amounts of potential nitrogen leaching in a two-factor split-plot experiment with the same sweet corn variety and soil type. It was found that the average relative error of the six treatments was 15.3%, which was an acceptable result compared with some reported similar studies of soil nitrogen leaching modeling (e.g., Wolf et al., 2005; Conrad and Fohrer, 2009), where the error could be as high as 71% or more.

Posterior Distribution of Parameters

The posterior distributions of parameters represent the uncertainty remaining in the parameters estimated for this study. This uncertainty depends on the parameter prior distributions as well as measurement uncertainties used in the GLUE procedure. It is interesting to compare the posterior distribution of parameters with their prior distributions (table 7), remembering that the prior distributions were based on parameters for many maize varieties in the DSSAT database that vary considerably in their characteristics and for many soils that also have a wide range of textures. In contrast, the posterior distribution represents the specific soil and maize variety in the field study. Mean parameter values in the posterior distributions were thus considerably different from the prior values, the ranges defined by the minimum and maximum values were reduced, and standard deviations were also reduced dramatically. For example, the prior mean value of genotype parameter P1 was 225, but it changed to 99 after the GLUE procedure. The initial range [110, 450] was narrowed to [78, 182], and the standard deviations of P1 for the prior and posterior distributions were 68 and 8, respectively. For genotype parameter PHINT, there are many PHINT values of 39 in the DSSAT database because, when the parameter was externalized for the first time, available cultivars were assigned a common PHINT value of 39. Thus, the prior distribution and uncertainty associated with this pa-

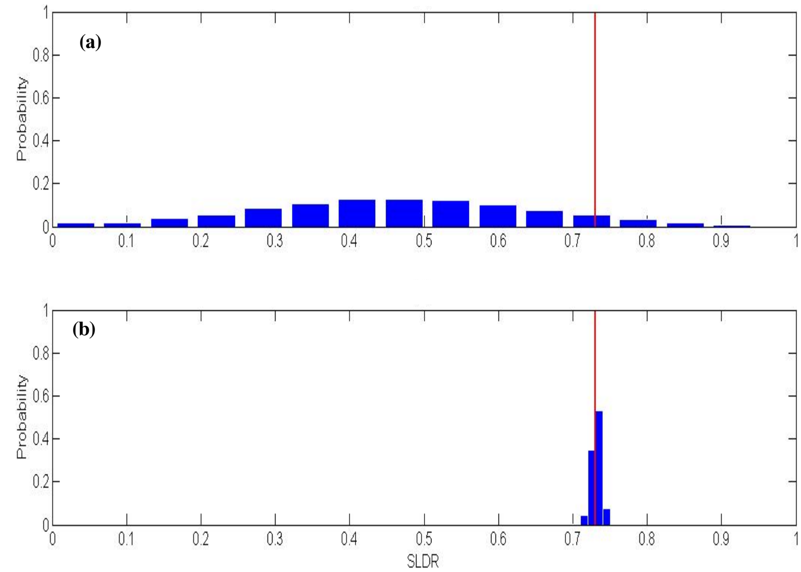

Figure 12. Parameter SLDR: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

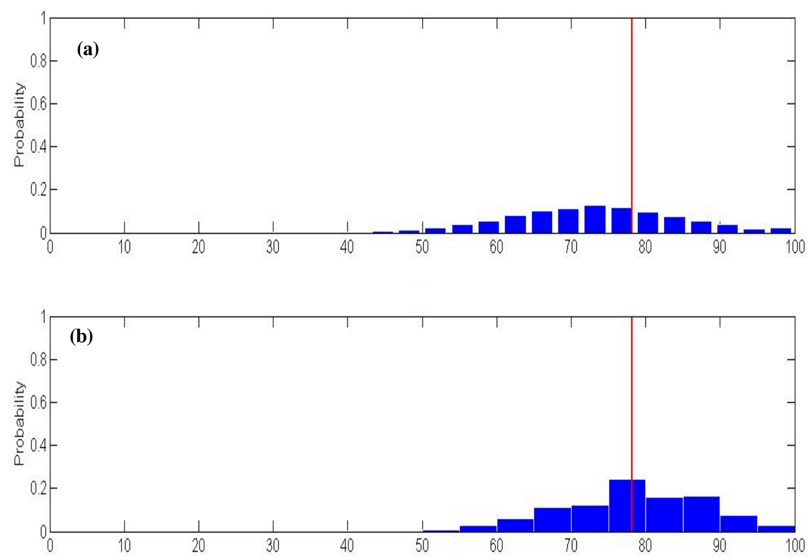

Figure 13. Parameter SLRO: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

rameter might have been affected by this dominance. In the prior distribution, the mean value of PHINT was 41.2, which was close to 39 compared to other available values such as 45 and 48. The values of standard deviation and CV were 4% and 10%, respectively. However, in the posterior distribution, the mean value of PHINT (40) became closer to the common PHINT value of 39, while the values of standard deviation and CV were significantly reduced to 0.2% and 0.5%, i.e., the uncertainty associated with this parameter was dramatically reduced. It can be concluded that the common PHINT value is a valid estimation for the sweet corn cultivar used in this study. Similar large changes were also found in other genotype and soil parameters. The CV values in posterior distributions all decreased to less than 10%, except for soil parameter SLRO.

The GLUE procedure resulted in different prior and posterior distributions of selected parameters (P1, P5, SLDR, SLRO, SLLL, and SDUL; figs. 10 through 15, respectively). The vertical lines show the estimated mean values of the parameters with the GLUE procedure. These figures reinforce that application of the GLUE procedure significantly reduced the uncertainty of model parameters and that the posterior means are good estimates of the parameters. After the two-step GLUE procedure, most of the posterior distributions followed normal distributions.

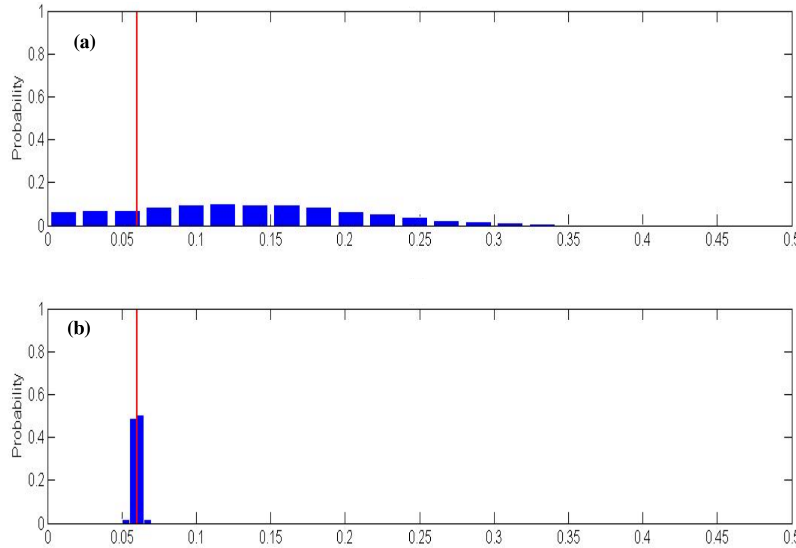

Figure 14. Parameter SLLL: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

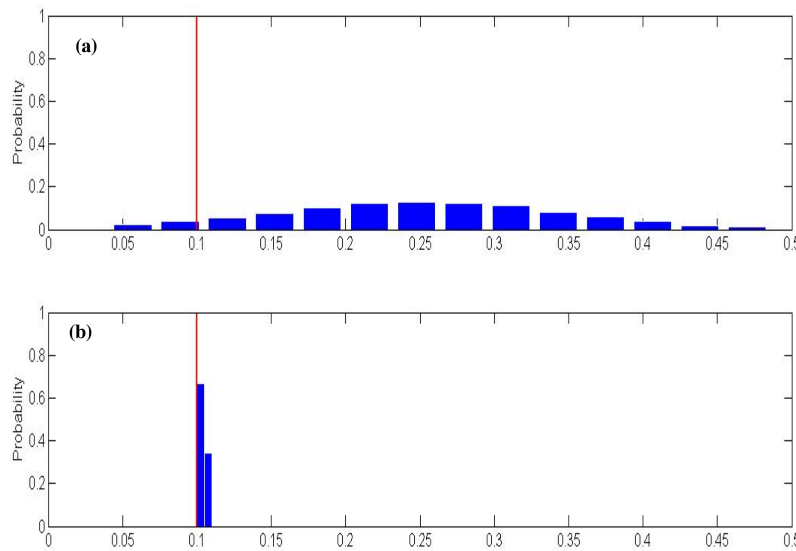

Figure 15. Parameter SDUL: (a) prior and (b) posterior distributions. Vertical line represents estimated mean parameter value.

Conclusions

In this study, the generalized likelihood uncertainty estimation (GLUE) method was used to estimate the genotype and soil parameters of the CERES-Maize model of DSSAT. Genetic coefficients (P1, P5, and PHINT) and soil parameters (SLDR, SLRO, SDUL, SLLL, and SSAT) were generated using a multivariate normal distribution that preserved the correlations between the parameters. The soil parameter SLPF was not correlated with other parameters and was generated with a uniform distribution.

After parameters were estimated, the CERES-Maize model correctly predicted the dry matter yields, anthesis dates, and harvest dates. The mean values of these variables were close to those measured in the field, with an average relative error of 4.4% and 2.4% for the data sets of 2005 and 2006, respectively. During the early stage of the growth season, the CERES-Maize model simulated the temporal trend of leaf TKN concentration accurately. However, the model underestimated the leaf TKN concentrations during the latter half of the season, which might be due to the mechanism of N content simulation in the model and fertigation events until late in the season.

The GLUE procedure accurately estimated soil parameters when compared with independent measurements made in the laboratory. Errors in SLLL, SDUL, and SSAT were 0.009, 0.006, and 0.014 $cm^3\ cm^{-3}$, respectively, an average absolute relative error of about 8.5%. The simulated time series of soil water content adequately simulated the observed soil water changes during both growth seasons for every layer. However, there were some substantial differences between simulated and observed soil nitrate contents, which were probably both due to the complexity of soil nitrogen dynamics modeling and the inaccuracy of the soil nitrate measurement techniques. Although the uncertainty in predicted potential nitrogen leaching was also significantly reduced through the GLUE method, in this research it cannot be concluded that the model correctly predicted the potential nitrogen leaching.

In the posterior distribution of estimated parameters, the uncertainties in parameters were substantially reduced, with CV values mostly lower than 10%. The average CV value of the parameters was reduced from 27% in the prior distribution to 5% in the posterior distribution. In general, the results of this study showed that the CERES-Maize model was capable of simulating sweet corn production in northern Florida along with the associated soil water dynamics. The model can also simulate potential nitrogen leaching with better accuracy than some reported similar studies, although there were some discrepancies in soil nitrogen prediction. It is suggested that the model can be used to compare different management practices relative to productivity and potential nitrogen leaching outcomes.

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