Estimating DSSAT Cropping System Cultivar-Specific Parameters Using Bayesian Techniques

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Abstract

Crop models are highly useful for simulating crop and soil processes in response to variations in climate and management. However, if one wishes to simulate a crop's performance in a specific soil and climate for a particular set of management inputs, cultivar-specific parameters (CSPs) are needed because of the genetic variations among cultivars of any crop. In this chapter, we summarized methods that have been used to estimate CSPs for the CERES and CROPGRO-based models in the Decision Support System for Agrotechnology Transfer (DSSAT) cropping system model. We primarily described a Bayesian parameter estimation procedure (the Generalized Likelihood Uncertainty Estimation, or GLUE) for use in estimating CSPs in DSSAT. The procedure is simple to use, requiring only that users select a crop, a cultivar, and the data for use in the estimation procedure from a list of data available for that cultivar in the DSSAT system. Results are displayed for users to view and copy to the standard cultivar file in DSSAT for the crop involved. The procedure does require a large number of model runs; we recommend 6,000 but users can optionally change this number.

Two cultivars ('Prisma' and 'Williams') of two crops (maize and soybean, respectively) were selected to demonstrate the performance of DSSAT GLUE program. For 'Prisma' maize, two experiments conducted in Zaragosa, Spain in 1995 and 1996 were selected; for 'Williams' soybean, three experiments individually conducted in Wooster, Ohio and Gainesville, Florida, were selected for the demonstration. Results showed that the GLUE method performed better than the arbitrary default CSPs and slightly better than the hand-calibrated CSPs in simulating these maize and soybean cultivars when using one time measurements, such as phenology dates, final dry matter yield, maximum leaf area index, and grain yield. For example, in the 'Prisma' maize experiments in Zaragosa, Spain in 1995 and 1996, the average relative absolute error (RAE) values between the simulated and measured output variables were only 3% and 8%, respectively, while they were between 4% and 10% for hand-calibrated CSPs and above 16% for the default CSPs.

Keywords: *Parameter estimation, Genetic coefficients, GLUE, DSSAT, Bayesian*

1. Introduction

Crop models are highly useful for simulating crop and soil processes in response to variations in climate and management. The basic concept is that simulating crop growth and yield using dynamic crop models will produce results that represent how a real crop growing under specific environment and management conditions would perform. Furthermore, if simulated results are sufficiently accurate, one can perform experiments using the models to evaluate likely responses to climate, soil properties, and crop and soil management. However, there are practical limitations that must be considered before making use of this approach in any study. One main limitation is that crop models do not contain all of the factors in the field that may influence crop yield. For example, crop diseases, weeds, and spatial variability of soils and management implementation can cause large differences in yield, and these factors are seldom included in crop simulation analyses. Another limitation is that inputs must be accurate or else simulated outputs are unlikely to match observations from the field. Attempts to evaluate the predictability of a crop model thus require that weather, management and soil inputs are measured in the field where the evaluation experiments are conducted. Furthermore, model evaluation experiments would ideally be designed to eliminate yield-reducing factors that are not included in the model. And finally, parameters that are used to model the dynamics of soil and crop processes need to be accurate for comparison with observed field data. For example, if one uses a crop model to simulate crop yield responses to water or N management using incorrect soil water parameters, results will show that the model fails to mimic results from field experiments or, more problematically, provide results that may mislead researchers or other model users.

If, however, one wishes to simulate crop growth and yield for large areas in which soils and climate vary, the input soil, weather, and management conditions should represent the spatial variability that exists over the area in order to provide reliable estimates at aggregate scales. In this case, many possible fields may be simulated without an attempt to mimic any particular real field. The objectives of such studies may be to compare aggregate effects of crops, varieties, and management systems under the range of soil and climate conditions that existing in an area. Options can be evaluated for changing crop management in an area to achieve a goal, such as to study management options for adapting to potential changes in climate. For these broad studies, model inputs need to represent the spatial variability that exists over the landscape and crop and variety parameters should accurately represent those of a particular field from which observations were collected for comparisons with the model.

In this chapter, we focus on methods for estimating parameters for the Decision Support System for Agrotechnology Transfer (DSSAT) cropping system model (Tsuji et al., 1994; Jones et al., 2003; Hoogenboom et al. 2003; Boote et al., 2003) using data collected from field studies on real cropping systems. When field observations are used to estimate model parameters, however, the resulting parameters may not be transferrable to other conditions. This model transferability depends on its robustness, the parameters used in model equations, and the quality of observations used as model inputs and response variables. Parameters in models are often highly related to their testing conditions and are less universal than expected. Therefore all crop models should be calibrated and validated for the environment of interest if results are to be credible (Timsina and Humphreys, 2006).

Emphasis is given to estimating the so-called genetic coefficients (Ritchie, et al, 1986; Hunt et al., 1993; Boote et al., 2003), or what are more accurately referred to as cultivar-specific parameters (CSPs). The implicit assumption in the models is that there are parameters for a given crop species that remain the same for all cultivars and that there are parameters that vary among cultivars and which allow simulating differences in yield or other traits when different cultivars are grown in the same environments and management conditions (Bertin et al., 2009; Boote et al., 2001). This is important because there are many existing cultivars and new ones are released each year. Because the CSPs are not known for most cultivars, model users need to estimate them using field data. The emphasis in this chapter on CSPs should not be interpreted as a statement that they are more important than soil parameters. As stated above, when one attempts to evaluate simulated results with field observations, soil physical and chemical properties and initial conditions are very important. In some cases, crop yield responses are more strongly affected by uncertainties in soil parameters than by CSPs (Jones et al., 2010; Mavromatis et al., 2001).

One should not expect a crop model to accurately simulate soil water and nutrient dynamics or growth and yield of a crop unless soil physical and chemical properties and CSPs are accurate. Methods presented in this chapter can also be used to estimate soil parameters if appropriate soil measurements are taken in the field where an experiment is conducted (He et al., 2009), but the procedure implemented in DSSAT only estimates CSPs. Furthermore, a model may not be sensitive to some of its parameters, and in such cases, one may need to put less effort into estimating those parameters than others. A sensitivity analysis is generally recommended before estimating parameters for models (e.g., see Jawitz et al., 2008; Monod et al., 2006; Makowski et al., 2006; Muñoz-Carpena et al., 2007 and 2010; Saltelli et al., 2004). However, we used prior experience to select the CSPs to estimate in the DSSAT implementation so it is not necessary for users to do this before using the DSSAT GLUE program.

The objectives of this chapter are to summarize methods that have been used to estimate CSPs for the CERES and CROPGRO-based models in DSSAT, and to present a Bayesian parameter estimation procedure (the Generalized Likelihood Uncertainty Estimation, or GLUE) that is in the latest release of DSSAT (v 4.5, Hoogenboom et al., 2010). Some results are presented to highlight the capabilities and limitations of this approach.

2 General Parameter Estimation Approaches

Model parameter estimation, sometimes referred to as calibration, is the process of estimating parameters to obtain a match between observed and simulated system behavior (Oliva, 2003). This requires a set of observed data from the real system, the model that simulates the system's behavior, a criterion for determining the best parameters, and a method to determine the best parameter set. Generally, the criterion is to minimize the error between observed and simulated variables. Many methods have been developed and used, such as conjugate gradient-descent search (Bhalla and Bower, 1993), stochastic-search (Foster et al., 1993), genetic algorithms (Baldi et al., 1998; Eichler-West and Wilcox, 1997; Vanier and Bower, 1996), and simulated annealing (Baldi et al., 1998; and Vanier and Bower, 1996). Perhaps the most common approach is trial and error (Wallach et al., 2001). Various parameter values are tested until a set of values is found that gives an acceptable fit to the data. For example, when Müller et al. (2003) calibrated the DAISY model to simulate decomposition of plant residues in soil, they used a stepwise trial and error process. The criterion of each iteration step was either to minimize the root mean square error (RMSE) or to maximize modeling efficiency (EF). The trial and error process has been criticized because it is unreliable and difficult to replicate (Lyneis and Pugh, 1996). Manual calibration may also be very tedious and time consuming, depending on the number of model parameters and the degree of parameter interaction. Thus, a great deal of research has been directed to development of more effective and efficient automatic calibration procedures (Madsen et al., 2002).

There are two general approaches used to estimate parameters, frequentist and Bayesian (Makowski et al., 2006). The frequentist approach uses estimation methods to approximate assumedly-true and fixed parameter values by using a sample of data. Prior information on parameter values are not taken into account. The use of a frequentist method gives a single, deterministic estimate of each parameter. In contrast, Bayesian methods estimate parameters from two types of information, a sample of data (like the frequentist method) and prior information about parameter values. The results of Bayesian methods are probability distributions of parameter values. All Bayesian methods proceed in two steps. The first step is to define a "prior" parameter probability distribution based on literature or expert knowledge. The second step involves calculating a new parameter probability distribution from both the prior distribution and the available data set. This new distribution, called the "posterior" distribution, is computed by using Bayes theorem (Makowski et al., 2006).

Bayesian methods are becoming increasingly popular for estimating parameters for complex mathematical models (e.g. Campbell et al., 1999) because it provides a coherent framework for dealing with uncertainty. This is also due to the increase in speed of computers and the development of new algorithms (Malakoff, 1999). One commonly used Bayesian method is the GLUE method (Beven and Binley, 1992; Franks et al., 1998; Shulz et al., 1999) mentioned before. The GLUE method assumes that, in the case of large models with many parameters, there is no exact inverse solution. Hence, the estimation of a unique set of parameters, which optimizes a goodness-of-fit criterion given the observations, is not possible (Romanowicz and Beven, 2006). The main principle of this method is to discretize the parameter space by generating a large number of parameter values from the prior distribution. Likelihood values are then calculated for each parameter set using field observations. Probabilities, an empirical posterior distribution of the parameters, are calculated using Bayes' equation.

Since it was introduced in 1992, the GLUE framework has found widespread application in environmental modeling (Blasone et al., 2008). The popularity of GLUE is largely due to its conceptual simplicity, relative ease of implementation and use, and its ability to handle different error structures and models without major modifications to the method itself (Blasone et al., 2008). Example applications include those for rainfall-runoff (Beven and Binley, 1992; Freer et al., 1996; Lamb et al., 1998), soil erosion (Brazier et al., 2001), tracer dispersion in a river reach (Hankin et al., 2001), groundwater and well capture zone delineation (Feyen et al., 2001; Jensen, 2003), unsaturated zone (Mertens et al., 2004), flood inundation (Romanowicz et al., 1996; Aronica et al., 2002), land-surface-atmosphere interactions (Franks et al., 1997), soil freezing and thawing (Hansson and Lundin, 2006), crop yields and soil organic carbon (Wang et al., 2005), ground radar-rainfall estimation (Tadesse and Anagnostou, 2005), and distributed hydrology (McMichael et al., 2006; Muleta and Nicklow, 2005). He et al. (2009 and 2010a) used the GLUE method to estimate soil parameters and CSPs in the DSSAT CERES-Maize model.

There are a number of other Bayesian methods for estimating parameters, including the Metropolis-Hastings method (Makowski et al., 2002). We implemented the Metropolis-Hastings method in one study and found that it is more difficult to implement, but more efficient than GLUE (Hu and Jones, 2010). The major difference between these methods is that the Metropolis-Hastings method uses a Markov Chain – Monte Carlo (MCMC) parameter search method whereas the GLUE method uses a Monte Carlo random search method. In this chapter, we present the GLUE method that is implemented in the latest release of the DSSAT software (version 4.5, Hoogenboom, et al., 2010).

3. Methods and Materials

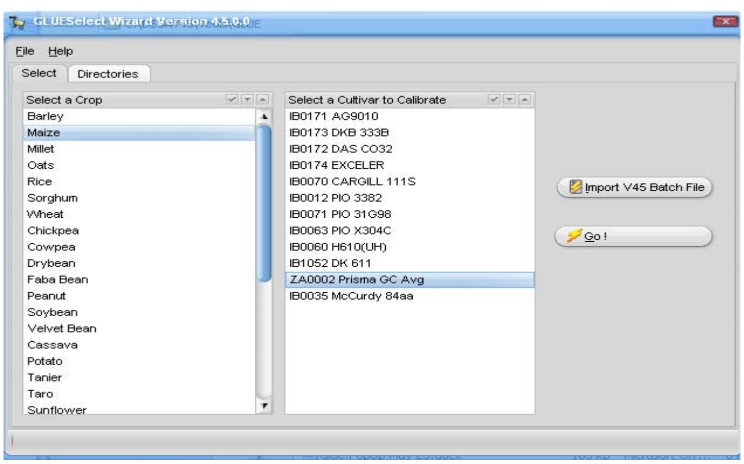
3.1 Overview of DSSAT

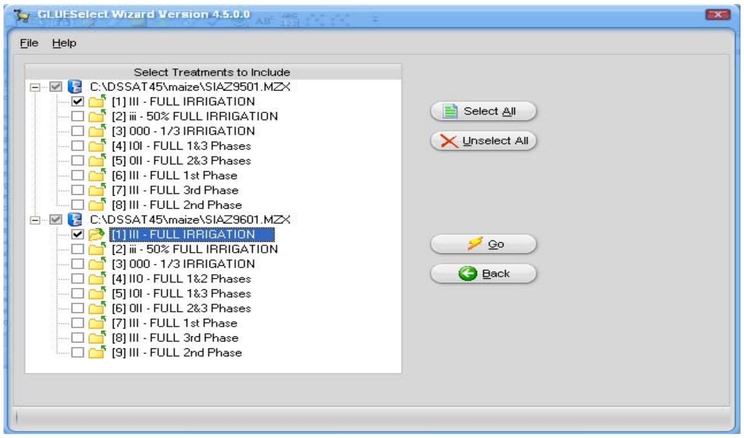
The DSSAT is a software system that combines crop models with observed data from field trials and tools that help users enter data from experiments, evaluate the models, estimate CSPs, conduct sensitivity analyses, analyze economic risk and uncertainty of alternative management options, and graphically present simulated and observed results (Uehara, 1998; Jones et al., 1998; Hoogenboom et al., 2003). One of the unique features of this system is that it has databases that connect to the crop models and are used for evaluating model performance and estimating CSPs. At the heart of DSSAT is the cropping system model (DSSAT- CSM), which incorporates all crops as modules using a single soil model (Jones et al., 2003). The DSSAT v 4.5 can simulate more than 20 crops, including maize (*Zea mays L.*), wheat (*Triticum aestivum* L.), rice (*Oryza sativa* L.), sorghum [*Sorghum bicolor* (L.) Moench], soybean [*Glycine max* (L.) Merr.], and peanut (*Arachis hypogaea*). The CSM simulates growth, development and yield of a crop growing on a uniform area of land under specified management. The dynamics of soil water, carbon, nitrogen and phosphorus that take place in the cropping system over time are also simulated. The model is structured using the modular approach described by Jones et al. (2001) and Porter et al. (2000) and consists of a main driver program, a land unit module, and primary modules for weather, management, soil, plant, and soil-plant-atmosphere interface components.

A number of methods have been used in the past to estimate CSPs for the different crops in the DSSAT-CSM. In many cases, trial and error methods are used to select a set of parameters that visually fits the observed data and/or produces an acceptably low RMSE between simulated and observed variables, often using a combination of time-series and end-of-season data concurrently (e.g., Boote, 1999; Boote et al., 2003). Other methods include the Simplex method (Grimm et al., 1993), Simulated Annealing (Mavromatis et al., 2001, 2002), and the K-Nearest Neighbor approach (Bannayan and Hoogenboom et al., 2008). A CSP estimation tool was developed by Hunt et al. (GENCALC, Hunt et al., 1993) and integrated into DSSAT v3.0, and v3.5. This tool automated a systematic search of parameters that minimized RMSE between simulated and observed variables; the criteria for selecting parameter values depended on the parameter being estimated in a sequential search process. A new updated version of this tool is also available in DSSAT v4.5.

3.2 Implementation of GLUE in DSSAT

The GLUE CSP estimation method was integrated into DSSAT using the R language (R Development Core Team, 2009; http://www.R-project.org), a free software environment for statistical computing and graphics. The program is simple to use in that users only have to select a crop, a cultivar (from a list of cultivars included in the DSSAT database for that crop), and the treatments from the various experiments in which that cultivar was grown (Fig. 1). The ranges of CSPs are stored in a file so that users do not have to specify these values. Optionally, users can choose to estimate only phenology CSPs, only growth CSPs, or both of them simultaneously, and set the number of runs to make. The interface also allows users to view the final estimated parameters and their distributions. The GLUE calculations are made using the GLUE R program, which calls the DSSAT CSM, connects the data to the model, generates all parameter sets, and performs all of the necessary calculations to select the CSPs.





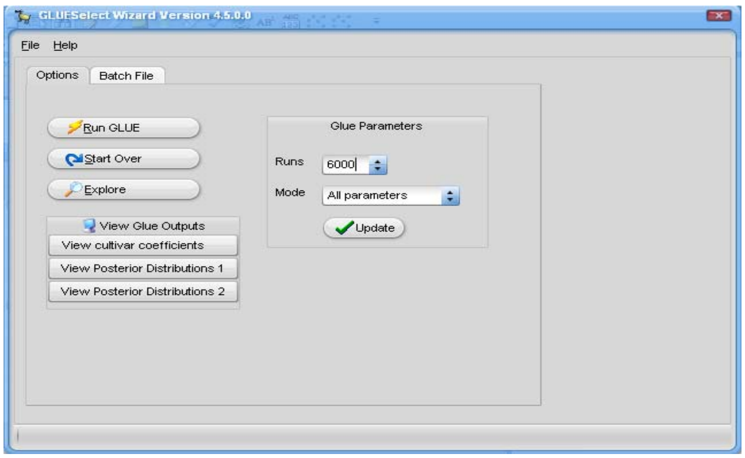


Figure 1. Screen shots of the DSSAT GLUE program user interface. Users first select a crop, then a cultivar (Fig. 1 top), then select which treatments they wish to use for estimating the CSPs (Fig. 1 middle), and then run the procedure in Fig. 1 (bottom). After the program finishes, users view the coefficients (Fig. 1 bottom) and can copy and paste the estimated CSPs into the crop cultivar file. Users may also view the standard deviations of CSP estimates from this last screen.

3.3 Theoretical Basis of the GLUE Method in DSSAT v4.5

Although users do not need to know all of the calculations that are done to arrive at the estimated CSPs when they use the GLUE program, we summarize the main theoretical basis for the method and the steps used internally in the program. In the GLUE procedure, a likelihood function is used as the criterion for estimating CSPs similar to that used by He et al. (2009). A likelihood value is computed for each observation, given each particular set of randomly-generated CSP sets. The Likelihood Function is the product of these individual likelihood values. In DSSAT, the Gaussian likelihood function (Equation 1) (Beven and Binley, 1992; Romanowicz et al., 1994, 1996; Makowski et al., 2002; He et al., 2009 and 2010a,b) was used:

$$L[\theta_i \mid O] = \prod_{j=1}^{M} \frac{1}{\sqrt{2\pi\sigma_o^{\,2}}} \exp\left(-\frac{\left(O_j - Y(\theta_i)\right)^2}{2\sigma_o^{\,2}} \right), \quad (i = 1,2,3\ldots N) \qquad (1)$$

where θ_i is the *i*-th parameter set; N is the total number of parameter sets generated by the program, $Y(\theta_i)$ is the model output using parameter set θ_i; O is the observation; O_j is the *j*-th observation of O; σ_o^2 is the variance of model error; and M is the number of observations.

The probability p_i of each parameter set is computed with the equation (He et al., 2009):

$$p(\theta_i) = \frac{L(\theta_i \mid Y)}{\sum_{i=1}^{N} L(\theta_i \mid Y)} \tag{2}$$

where $p(\theta_i)$ is probability or likelihood weight of the *i*-th parameter set θ_i, and $L(\theta_i \mid Y)$ is the likelihood value of parameter set θ_i, given observations Y.

The GLUE methodology (Beven and Binley, 1992) thus develops an approximate discrete posterior probability distribution, designated by (θ_i, p_i), $i = 1,...,N$, $\sum_{i=1}^{N} p_i = 1$, where p_i is the probability associated with the parameter vector θ_i, and N is the total number of generated parameter vectors.

Equations (1) and (2) are used to construct the posterior distributions of the CSPs. The implementation in DSSAT uses two iterations of GLUE, one to estimate phenological development parameters and the others to estimate growth parameters. This was done for practical reasons, mainly due to the time required when estimating all parameters simultaneously. This can be done in the DSSAT models because development is largely independent of growth but not vice versa. Thus, the development parameters are first estimated followed by those that affect biomass growth and yield in a 2-step sequence. Thus, there are two posterior distributions, one for each step.

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

(1) *Develop prior parameter distributions*. In this study, the CSPs of two crops (maize and soybean) in the DSSAT database (Hoogenboom et al., 2003) were analyzed to determine the prior range of each parameter. Because we do not have additional information, the prior distributions are assumed to be independent and uniformly distributed between the minimum and maximum values across all cultivars previously calibrated for each crop.

(2) *Generate random parameter sets from the prior parameter distributions*. A large number (e.g., 6,000) parameter sets are created by randomly generating each CSP in each of 6,000 CSP vectors independently, according to the prior uniform distribution of each CSP. The number of runs can be modified by the user, but at least 3,000 runs are recommended (He,

2008) to ensure that CSPs are each estimated accurately and the calculated posterior distributions are reliable.

(3) *Run the model with the randomly-generated parameter sets.* The model is run with the parameter sets generated above. The standard genetic input file is changed to simulate every random parameter set in sequence. Model outputs (including anthesis date, maturity date, dry matter yield, leaf area index, leaf number etc., which could be selected by model users) for each parameter set are tabulated for use in the GLUE likelihood calculations.

(4) *Calculate the likelihood values*. The observations (Y) from the selected data provided by model users are used along with the corresponding simulated outputs to compute the likelihood value, $L(\theta_i \mid Y)$, for each generated parameter vector θ_i .

(5) *Construct posterior distribution and statistics*. The pairs of parameter sets and probabilities, $(\theta_i, p_i), i = 1,..., N$, are computed and used to construct the posterior distribution and to compute the mean, and variance of the selected parameters using following equations:

$$\hat{\mu}_{post}(\theta) = \sum_{i=1}^{N} p(\theta_i) \cdot \theta_i \tag{3}$$

$$\hat{\sigma}^2{}_{post}(\theta) = \sum_{i=1}^{N} p(\theta_i) \cdot (\theta_i - \hat{\mu}_{post})^2 \tag{4}$$

where $\hat{\mu}_{post}(\theta)$ and $\hat{\sigma}^2{}_{post}(\theta)$ are the estimated mean, variance of the posterior distribution of parameters θ ; $p(\theta_i)$ is the probability of the *i*-th parameter set θ_i calculated by Equation (1); and N is the number of random parameter sets.

3.4. Application of GLUE to Estimate CSPs of Maize and Soybean

CSPs were estimated for maize and soybean to demonstrate the method’s performance and characteristics of results that were obtained. In particular, we show observed and simulated values derived from the CSPs selected using the GLUE method. We also present uncertainties in the estimated CSPs and in simulated outputs.

Table 1 lists the CSPs of the CERES-Maize model in DSSAT (Jones et al., 2003) that are estimated in the GLUE procedure. The CSPs P1, P2, and P5 determine the timing of phenological events, such as anthesis date and maturity date of maize. Coefficients G2 and G3 control the yield-related outputs, such as grain dry matter yield, grain size, canopy weight, etc. Our 2-step procedure requires that all CSPs estimated in the first step be completely determined by phenological development data. The CSPs estimated in the first step plus all other CSPs in the second step affect growth responses. Phenological development is assumed to be independent from growth in the model, but growth is affected by phenological development. This assumption is reasonable unless major stresses occur. The CERES-Maize

CSP PHINT is not included in the procedure because its value is similar across many cultivars and because it influences both phenological development and yield. PHINT was assumed to be 48.0 for all cultivars.

Table 1. Cultivar-specific parameters in the DSSAT CERES-Maize model (Jones et al., 2003) that are estimated in the DSSAT GLUE procedure

Coefficient	Minimum	Maximum	GLUE Flag [1]	Definition
P1	140	365	1	Degree days (base 8 ^oC) from emergence to end of juvenile phase
P2	0.0	1.0	1	Photoperiod sensitivity coefficient (0-1.0)
P5	600	990	1	Degree days (base 8 ^oC) from silking to physiological maturity
G2	500	908	2	Potential kernel number
G3	5	15	2	Potential kernel growth rate mg/(kernel d)

[1]GLUE flag is an indicator to show in which round of the procedure the parameter will be estimated.

Table 2 shows the CSPs for the CROPGRO-Soybean model in the DSSAT-CSM. There are 18 total CSPs in soybean (Boote et al., 2003), but the eleven coefficients in the table below are those that vary most among cultivars and determine differences in soybean cultivars' responses to their environments. The model is highly sensitive to these CSPs and less sensitive to the other ones when they are near their nominal values in the cultivar file available in DSSAT.

Table 2. Cultivar-Specific Parameters for the soybean crop in the DSSAT-CSM (from Boote et al., 2003) that are estimated in the GLUE procedure.

Coefficient	Minimum	Maximum	GLUE Flag [1]	Definition
CSDL	11.78	14.6	1	Critical Short Day Length below which reproductive development progresses with no day length effect (for short day plants) (h)
PPSEN	0.129	0.349	1	Slope of the relative response of development to photoperiod with time (positive for short day plants) (1/h)
EM-FL	15.5	23.5	1	Time between plant emergence and flower appearance (R1) (PTD [2])
FL-SD	12	16	1	Time between first flower and first seed (R5) (PTD)
SD-PM	29.5	37.5	1	Time between first seed (R5) and physiological maturity (R7) (PTD)
LFMAX	1	1.4	2	Maximum leaf photosynthesis rate (at 30C, 350 vpm CO_2, high light, mg CO_2 m^2 s^{-1})
SLAVR	350	425	2	Specific leaf area of cultivar under standard growth conditions (cm^2 g^{-1})
SIZELF	140	230	2	Maximum size of full leaf (three leaflets) (cm^2)
WTPSD	0.155	0.195	2	Maximum weight per seed (g)
SFDUR	17	25.5	2	Seed filling duration for pod cohort at standard

				growth conditions (PTD)
SDPDV	1.7	2.44	2	Average seed per pod under standard growing conditions (no. pod^{-1})

[1]GLUE flag is an indicator to show in which round of the procedure the parameter will be estimated.
[2]PTD, photothermal days, comparable to calendar days if at optimum temperature and CSDL.

In this chapter, two cultivars ('Prisma' and 'Williams' shown in Table 3) of two crops (maize and soybean, respectively) were selected as examples to evaluate the performance of DSSAT GLUE program. For 'Prisma' maize, the experiments conducted in Zaragosa, Spain in 1995 and 1996 were used. There are a total of 8 and 9 treatments based on different irrigation levels in 1995 and 1996, respectively, but only the fully irrigated treatments were selected so that development and growth were influenced only by weather, not due to water or nutrient stresses. Similarly, three experiments, which were conducted individually in Wooster, Ohio and Gainesville, Florida, were selected for 'Williams' soybean. Only irrigated treatments were used to estimate the CSPs. A summary of experimenal treatment characteristics, including planting date, N application, irrigation, and available observations is presented in Table 3.

Table 3. Summary of experiment details for the example maize and soybean cultivars and experiments in DSSAT v4.5 used for estimating Cultivar-Specific Parameters in this study (Hoogenboom et al. 2010). Also shown are the field observations used in each experiment.

Crop	Cultivar	Experiment	Experimental Items	Details
			Treatment	Full Irrigated
			Location	Zaragosa, Spain
		Zaragosa, Spain 1995	Planting date	5/17/1995
			N fertilizer	100 and 200 kg urea-N ha^{-1}
			Irrigation	A sum of 568 mm water in 9 events
			Available Observations	ADAP, MDAP, HWAM, HWUM, CWAM, LAIX [1]
Maize	Prisma			
			Treatment	Full Irrigated
			Location	Zaragosa, Spain
		Zaragosa, Spain 1996	Planting date	5/16/1996
			N fertilizer	100 and 200 kg urea-N ha^{-1}
			Irrigation	A sum of 505 mm water in 8 events
			Available Observations	ADAP, MDAP, HWAM, HWUM, CWAM, LAIX
			Planting date	5/1/1988
		Wooster, Ohio 1988	N fertilizer	No N applied.
			Irrigation	A sum of 595 mm water in 18 events
			Available Observations	ADAP, PD1P, MDAP, HWAM, HWUM, CWAM, LAIX,
Soybean				
			Planting date	4/30/1990
			N fertilizer	No N applied.
	Williams	Wooster, Ohio 1990	Irrigation	Not Irrigated (not necessary)
			Available Observations	ADAP, PD1P, MDAP, HWAM, HWUM, CWAM, LAIX

	Gainesville, Florida 1979	Planting date	3/15/1979
		N fertilizer	No N applied.
		Irrigation	A sum of 144 mm water in 14 events
		Available Observations	ADAP, PD1P, MDAP, HWAM,, HWUM, CWAM, LAIX

[1] These abbreviations represent the model output variables in DSSAT: ADAP=Anthesis date (days after planting), MDAP=Maturity date (days after planting), HWAM=Yield at harvest maturity (kg [dm]/ha), HWUM=Unit wt at maturity (g [dm]/unit), CWAM=Tops weight at maturity (kg [dm]/ha), LAIX=Maximum Leaf area index, PD1P=First pod day (days after planting), PWAM=Pod/Ear/Panicle weight at maturity (kg [dm]/ha).

The monthly average weather data were summarized for growing season months for these five different experiments (Table 4). Generally, solar radiation was higher and rainfall (mm d^{-1}) was lower for this maize experiment site than the other sites. Relatively, the Gainesville, FL, 1979, experiment had higher minimum and maximum temperatures and lower rainfall, which is due the subtropical climate of Florida. In the Ohio soybean experiments, solar radiation was higher and rainfall less than in Florida. Because irrigation was used in all of the experiments, water stress likely did not reduce yields relative to the potential yields.

Table 4. Monthly average weather data of the five experiments of maize and soybean (Hoogenboom et al. 2010).[1]

	Month	Apr	May	Jun	Jul	Aug	Sep	Oct
Zaragosa, 1995	Tmin	5.1	10.9	14.0	17.2	16.7	11.7	9.4
	Tmax	21.1	24.8	27.4	32.8	30.0	24.0	24.2
	Rain	2.0	1.2	0.3	0.1	0.5	0.3	0.1
	SRAD	22.1	21.5	25.1	25.6	22.9	17.8	12.5
Zaragosa, 1996	Tmin	6.4	10.0	14.3	15.9	16.0	11.8	8.1
	Tmax	19.3	23.2	28.4	30.5	28.7	24.2	20.4
	Rain	1.2	1.6	0.6	1.0	1.1	0.3	0.2
	SRAD	20.4	23.0	25.9	25.7	21.4	17.3	12.5
Wooster, Ohio 1988	Tmin	3.8	7.6	10.7	15.9	16.3	10.6	-
	Tmax	16.6	23.1	28.3	32.2	29.0	23.4	-
	Rain	1.9	1.1	0.4	5.2	2.8	2.5	-
	SRAD	15.0	20.3	23.9	20.3	18.0	13.6	-
Wooster, Ohio 1990	Tmin	7.3	13.2	15.5	14.6	11.2	5.6	-
	Tmax	19.6	25.7	27.4	26.8	22.9	17.7	-
	Rain	4.2	2.0	5.5	3.7	3.7	3.9	-
	SRAD	17.4	20.7	20.1	16.7	13.1	9.5	-
Gainesville, Florida 1979	Tmin	15.1	17.0	20.1	22.6	-	-	-
	Tmax	28.2	30.0	32.6	34.0	-	-	-
	Rain	6.9	2.8	3.9	3.6	-	-	-
	SRAD	19.1	21.3	20.4	21.1	-	-	-

[1] "Tmin"=minimum temperature (^{o}C), "Tmax"=maximum temperature (^{o}C), "Rain"=average daily rainfall (mm), and "SRAD"=solar radiation ($MJ/m^2/d$).

The CSPs estimated using the GLUE procedure were compared with those from two other sources—an arbitrary default set of CSPs used to initialize the GLUE procedure and the hand-calibrated CSPs that were in the DSSAT v4.5 cultivar database. Field observations from the selected experiments (Table 3) in DSSAT were compared with the model-simulated output variables derived from the three sources of CSPs. The relative absolute error (RAE percentage; Equation 5) was used as a measure to evaluate the differences between simulated and observed variables for each set of CSPs:

$$RAE = \frac{\left|\hat{Y} - Y\right|}{Y} \times 100\% \tag{5}$$

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

4. Results and Discussions

4.1 Maize Results

Comparison of simulated and observed crop variables. A comparison of results between field observed and model simulated output variables of 'Prisma' maize from three different sources of CSPs is summarized in Table 5. The GLUE-estimated CSPs did a better job than the arbitrary generic maize cultivar default CSPs and performed as well as the hand-calibrated CSPs in simulating this maize cultivar. The average RAE values were only 3% and 8% in 1995 and 1996, respectively, while they were 4% and 10% for the hand-calibrated CSPs and above 15% for the default CSPs. Using both the GLUE-estimated and hand-calibrated CSPs, the maize model predicted phenology dates very well. In 1995, there were 0 and 2 days differences between the GLUE simulated and observed anthesis and maturity dates respectively, while these values were 1 and 2 days in 1996. Results for the hand-calibrated CSPs were similar. However, the errors in phenology dates simulations with the default CSPs were high. For example, the anthesis and maturity dates simulated with Default CSPs were 11 and 18 days sooner than the field observations in 1996. Although the hand-calibrated CSPs for this cultivar performed about as well as the GLUE-estimated CSPs, it is dangerous for users to automatically use CSPs for a particular cultivar they are interested in without evaluating them for their own conditions, even if the cultivar's parameter set is contained in the DSSAT data base. Data from regions or locations where the model is to be applied should be used to evaluate simulated results relative to observations or used to estimate a new set of CSPs.

The average absolute error (RAE) between simulated and observed data was lower in 1995 for the GLUE-estimated CSPs (3%) than for the Default or Hand-Calibrated CSPs (17% and 4%, respectively) (Table 5). In addition, the RAE values were lower for all but one variable (biomass) when GLUE-estimated parameters were used in 1995 and 1996. In 1996, the GLUE-estimated parameters performed better on average as well; the RAE was 8% in comparison with 16% and 10% for Default and hand-calibrated CSPs, respectively.

Comparison of CSPs from GLUE with hand-calibrated and default CSPs. The parameter values of 'Prisma' maize obtained from different sources were compared (Table 6). There were large differences among the values of P1 and P2, which determine the thermal time of the vegetative and reproductive stages of maize. Thus, it is not surprising to see large differences among the predicted anthesis and maturity dates with these different sources of CSPs. The standard deviations were mostly less than 10% of the estimated CSPs (Table 6). An exception was for the parameter P2, the photoperiod sensitivity coefficient, which was nearly 40% of the estimated value. This is one indication that the model was not sensitive to this CSP for these two experiments, which was apparently due to the fact that the experiments were in the same location both years and there was little difference in daylengths that the two crops experienced.

Comparing in-season simulated results. Although time series data were not used to estimate CSPs in the GLUE procedure, we show time-series model outputs of in-season predictions for the three sources of CSPs for one season of 1995 (Fig. 2). In the maize experiments, no in-season data were collected, so it is not possible to draw conclusions about how well each set of CSPs performed in this example. However, it is interesting to show how different the in-season results are for two reasons. First, it is clear that similar or the same end of season simulations can be obtained with different CSPs, but that considerable differences may occur among in-season results. This can be seen in the GLUE simulated end point results for biomass and grain yield in Fig. 2. Secondly, in-season measurements may be very useful to refine the CSPs so that they simulate the time courses of growth and yield during a season. The differences among the simulated values of leaf area index (LAI) and grain weight (kg ha^{-1}) can be seen clearly.

4.2 Soybean Results

Comparison of simulated and observed crop variables. Similarly, comparisons of the results for 'Williams' soybean are tabulated in Table 7 for observed and simulated output variables for the three experiments in two locations. The GLUE and hand-calibrated RAE results averaged across all measurements were nearly equal. In about half of the RAE values for individual measurement variables, the GLUE method performed better and in the other half, the hand-calibrated CSPs performed better. For soybean, Dr. K. J. Boote of the Agronomy Department of the University of Florida (personal communication) estimated the CSPs using both end of season and phenology data with considerable emphasis on in-season measurements. Thus, the GLUE method did a good job in estimation of CSPs, since the average RAE values were equal to the "hand calibrated" CSPs and clearly less than most those of "default" CSPs. One exception was the maximum LAI (MaxLAI), for which the RAE obtained from the GLUE-estimated CSPs was 31%. The GLUE method also improved the accuracy of phenology date predictions relative to the other sources of CSPs. The differences between observed and GLUE simulated anthesis and maturity dates were all less than 2 days, except for the maturity date of the experiment in Gainesville, FL, in 1979, which was about 6 days.

Table 5. Comparison between observations and model output variables of ‘Prisma’ maize grown at Zaragosa, Spain

Source of Outputs	Phenology: Anthesis (d)		Phenology: Maturity (d)		Grain Yield (kg/ha)		Aboveground Biomass (kg/ha)		Max LAI		Average
	Value	RAE [1]	Value	RAE	Value	RAE	Value	RAE	Value	RAE	RAE
Zaragosa, Spain in 1995											
Field observations	78	-	141	-	10,960	-	23,970	-	6.15	-	-
Default CSPs	62	21%	113	20%	12,679	16%	26,428	10%	5.19	16%	17%
Hand-Calibrated CSPs	78	0%	141	0%	10,255	6%	25,648	7%	5.61	9%	4%
GLUE Calibrated CSPs	78	0%	139	1%	10,866	1%	26,437	10%	5.65	8%	3%
Zaragosa, Spain in 1996											
Field observations	78	-	147	-	12,340	-	22,730	-	4.75	-	
Default CSPs	67	14%	129	12%	13,626	10%	28,973	27%	5.69	20%	16%
Hand Calibrated CSPs	79	1%	151	3%	10,202	17%	25,327	11%	5.55	17%	10%
GLUE Calibrated CSPs	79	1%	149	1%	10,791	13%	26,079	15%	5.56	17%	8%

[1] The RAE values are the relative absolute error between field observed and model simulated variables from three different sources of CSPs.

Table 6. Comparison between cultivar-specific parameters (CSPs) of ‘Prisma’ maize.

Source of CSPs	P1	P2	P5	G2	G3
Default	200.0	0.300	800.0	700.0	8.50
Hand calibrated	280.0	0.300	789.0	650.0	6.03
GLUE calibrated values	268.2	0.758	770.8	675.1	6.439
(standard deviations)	(18.45)	(0.291)	(35.72)	(59.47)	(0.234)

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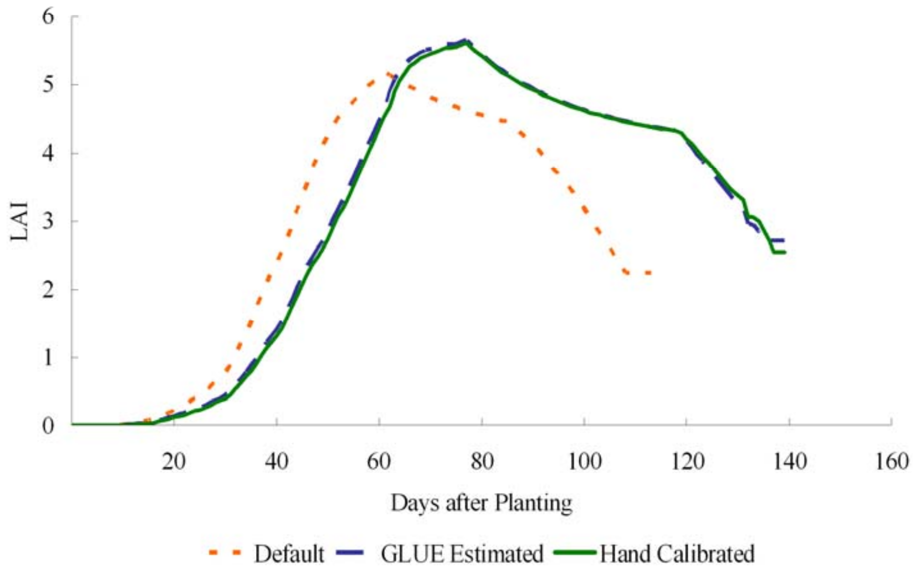

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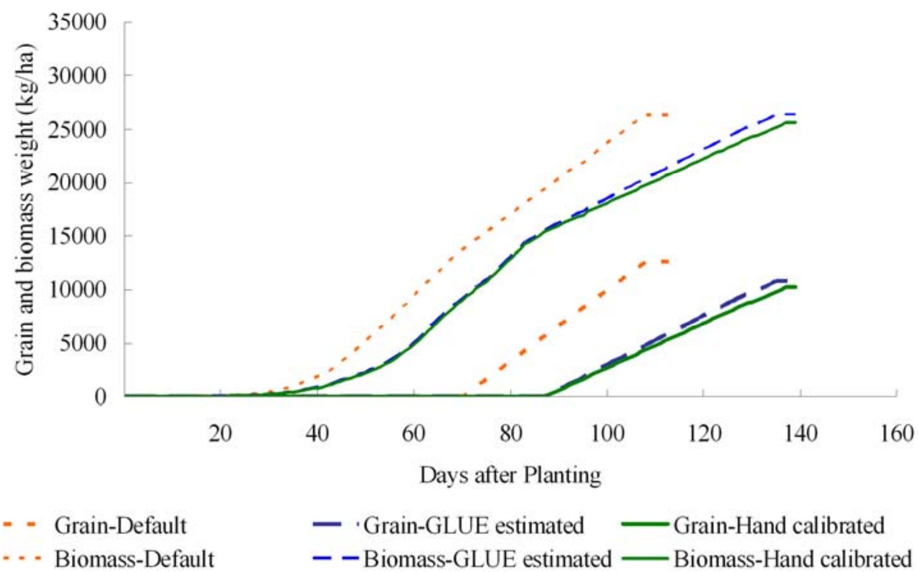

Figure 2. Graphs of simulated results using the three sources of CSPs for a) leaf area index, and b) total biomass and grain yield for the experiment in Zaragosa, Spain in 1995. ‘Default’ represents the outputs from default genetic coefficients; ‘GLUE estimated’ represent the outputs from GLUE estimated genetic coefficients; and “Hand calibrated” represent the outputs from hand calibrated genetic coefficients.

<u>Comparison of CSPs from GLUE with hand-calibrated and default CSPs.</u> The parameter values of 'Williams' soybean obtained from different sources are compared in Table 8. The default CSPs were assumed to be those of a generic maturity 4 soybean variety from the DSSAT database. Except for parameters SLAVR and SIZELF, the differences between these three types of CSPs were very small. The largest relative differences between Hand-calibrated and GLUE estimated CSPs were for PPSEN (0.285 vs. 0.342, respectively). The values of CSDL and PPSEN for Williams in Hand-calibrated CSP were not hand-calibrated, in fact, but were estimated using a least squares simplex method from a much larger (n>100) data set (Grimm et al., 1993). Thus, the GLUE-estimated photoperiod sensitivity coefficient (PPSEN) was obtained from a much smaller set of environments and is less robust across regions than that obtained by Grimm et al. (1993) for the hand-calibrated CSPs. This highlights a fundamental issue that transcends methods for calibration – that CSPs estimated from field data may not be robust if the size of the dataset used is small. Other relatively large differences occurred for SLAVR and SIZELF. Nevertheless, the standard deviations of the GLUE estimated CSPs were relatively low, indicating that the parameters worked well across the locations and years for this soybean cultivar.

<u>Comparison of in-season simulated and observed soybean results</u>. The time-series model outputs were also compared for 'Williams' soybean cultivar (Figs 3-5). All three experiments in this study provided field observations for some time-series output variables, such as LAI, biomass, and grain weight. These observations can help us to evaluate the reliability of the predictions from different CSPs sources. Most model outputs simulated using the "GLUE-estimated" and "hand-calibrated" CSPs were similar for all variables that were measured during the growing season. This result provides strong evidence that the GLUE method provided reliable CSP estimates, similar in performance to those that were estimated by an expert. However, this result also demonstrates the concept of "equifinality" (Beven and Freer, 2001; Hasson and Lundin, 2006; Shulz et al., 1999), which means that different combinations of CSPs will result in the same quality of simulation. The values of the GLUE CSPs were different from those estimated by K. J. Boote, yet simulated results and errors in prediction were nearly equal showing that different "best" CSP sets might exist. However, the GLUE-estimated CSPs did not correctly predict LAI for the Gainesville, FL 1979 experiment. It is not surprising to see that the GLUE method did not improve time-series prediction because there were no time-series observations involved in estimating the CSPs in the GLUE approach used in this study.

5. Conclusions

The use of field observations to estimate CSPs of cropping system models is necessary for practical uses in predicting crop performance under different soil, climate, and management scenarios. Various methods can be used to estimate CSPs, each with advantages and disadvantages. We presented the GLUE method in this chapter that has been implemented for estimating CSPs for all crops in DSSAT v4.5, using field observations made once during a season. We showed that this method works well for two of the crops in DSSAT. However, there are important theoretical considerations that users should be aware of when using any method to estimate CSPs using field data. First, any calibration process may result in CSPs that are not generally applicable, particularly if the range of environments in which data were collected is narrow or if the crops experience drought, nutrient, or other stresses that are not adequately simulated by the model. In the first situation, having a narrow range of environments may result in parameters that work well only for those environments. For example, if datasets with a narrow range of daylengths are used, the CSPs that determine photoperiod response in soybean (CSDL and PPSEN) are not likely to be robust for use across locations with daylengths outside that range. In the second situation, it is likely that the estimation process will attempt to set CSP values to compensate for water, nutrient, or pest stresses if they occur and are not adequately simulated in the model. This problem can happen when the model does not include mechanisms for simulating those stresses, or when the soil parameters or initial conditions are not accurate. This is a main reason for recommending the use of irrigated and well-fertilized treatments for estimating CSPs. This is true for the GLUE and GENCALC methods available in DSSAT as well as any other procedure where the two described situations occur. Another principle that is important regardless of method used is that the model itself may not adequately represent the crop development and growth processes adequately. In this case, one may obtain estimates from a particular set of field data that work well for that set of data but may not be robust. Thus, it is important for users to evaluate any existing CSPs for their own conditions if they were estimated in other environments.

In this chapter, two cultivars were selected, one for each of two crops (maize and soybean), to evaluate the performance of GLUE program. It was shown that the GLUE estimated CSPs for maize were different from the default values and from the manually estimated parameters. Similarly, the soybean CSPs estimated by the GLUE procedure were different from the arbitrary default set. However, soybean CSPs were similar to those manually estimated by an expert model user. Simulated outputs using the GLUE-estimated CSPs and hand-calibrated CSPs were similar to observed maize values. Both compared more favorably to observed maize values than those obtained from the default CSPs. For soybean, the simulated outputs were superior to the default set and equivalent to those obtained using the hand-calibrated CSPs. The average RAE values were all smaller than those for default set and generally equal to those for hand calibrated CSPs in this study. There are limitations of the GLUE program as implemented in DSSAT. First, it does not include time-series measurements. As shown in the comparisons time-series observations, the GLUE method did not always improve the accuracy of in-season model predictions but it also did not deteriorate accuracy. This limitation can be overcome in future implementations of methods to estimate CSPs. Secondly, the GLUE program requires a large numbers of model runs, which may require more than one hour on modern microcomputers. Nevertheless, implementation of the GLUE procedure in DSSAT v4.5 provides users an easy to use option for estimating CSPs from field observations for cultivars grown in their region.

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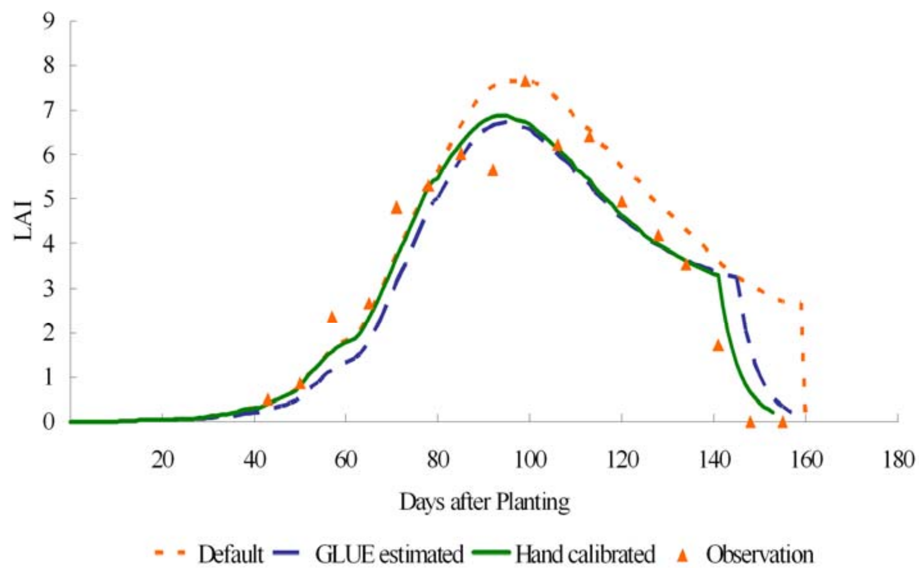

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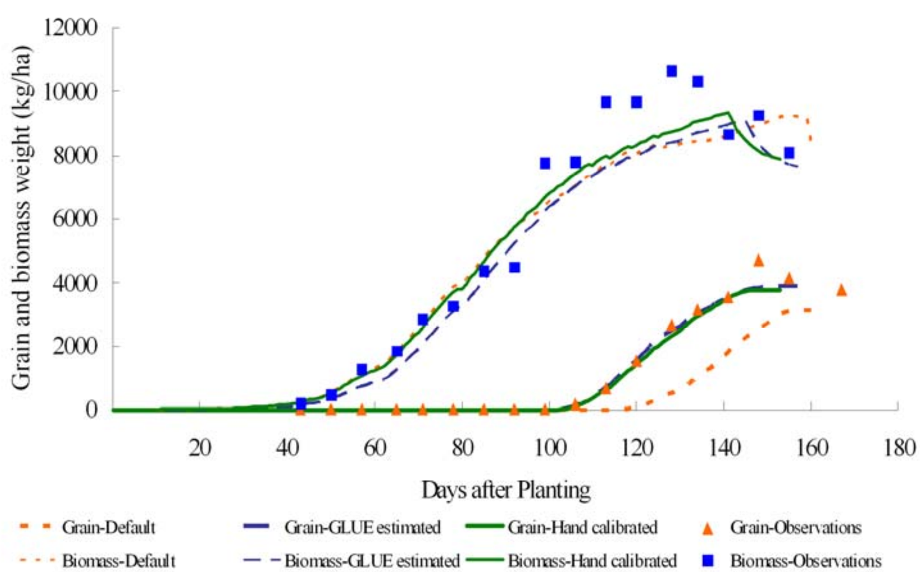

Figure 3. Graphs of observed and simulated results using the three sources of CSPs for a) leaf area index, and b) total biomass and grain yield for the experiment in Wooster, Ohio in 1988. 'Default' represents the outputs from Default genetic coefficients; 'GLUE estimated' represent the outputs from GLUE estimated genetic coefficients; and "Hand calibrated" represent the outputs from hand calibrated genetic coefficients by K.J. Boote.

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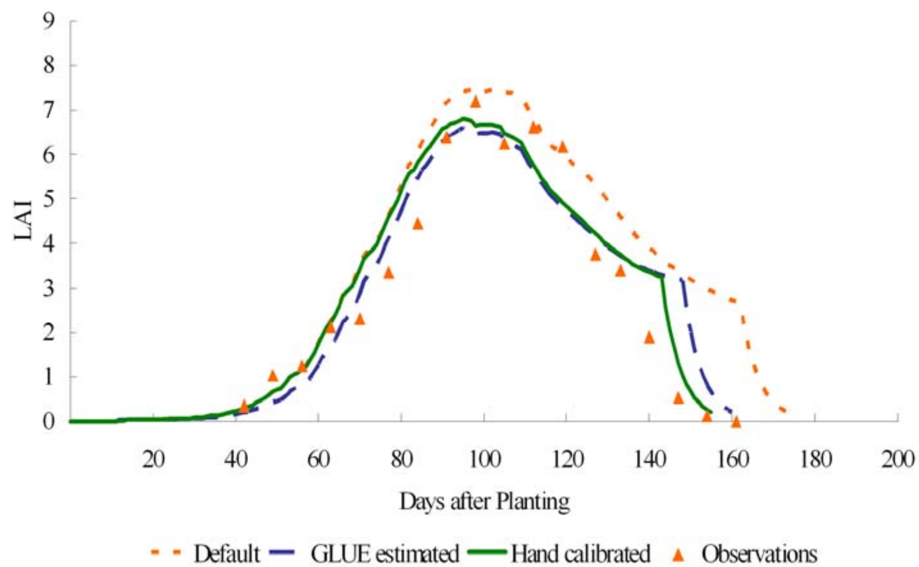

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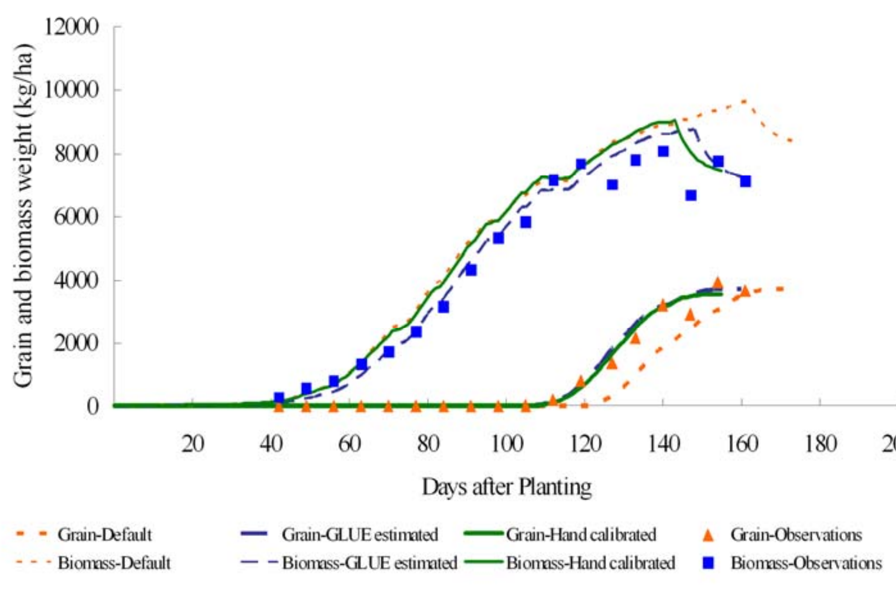

Figure 4. Graphs of observed and simulated results using the three sources of CSPs for a) leaf area index, and b) total biomass and grain yield for the experiment in Wooster, Ohio in 1990. 'Default' represents the outputs from Default genetic coefficients; 'GLUE estimated' represent the outputs from GLUE estimated genetic coefficients; and "Hand calibrated" represent the outputs from hand calibrated genetic coefficients by K.J. Boote.

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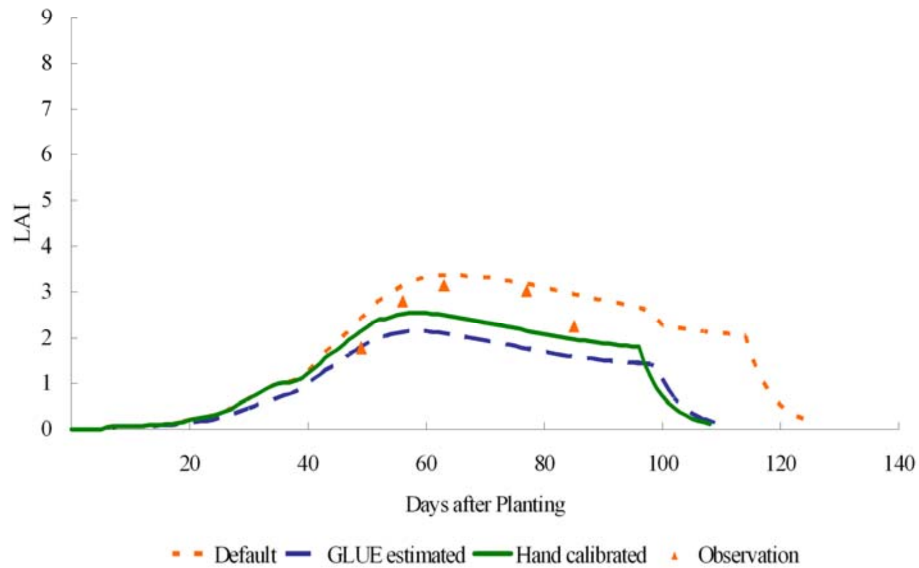

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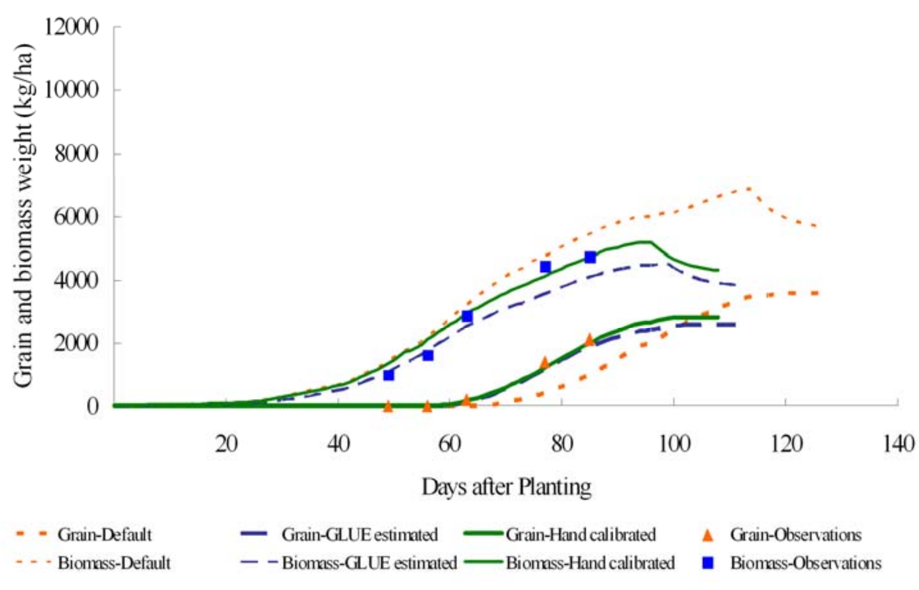

Figure 5. Graphs of observed and simulated results using the three sources of CSPs for a) leaf area index, and b) total biomass and grain yield for the experiment in Gainesville, FL in 1979. 'Default' represents the outputs from Default genetic coefficients; 'GLUE estimated' represent the outputs from GLUE estimated genetic coefficients; and "Hand calibrated" represent the outputs from hand calibrated genetic coefficients by K.J. Boote.

Table 7. Comparison between observations and model output variables of 'Williams' soybean. Default CSPs are those for "generic" MG 4 cultivar.

Source of Outputs	Phenology								Aboveground							
	Anthesis (d)		Maturity (d)		Grain Yield (kg/ha)		Biomass (kg/ha)		Max LAI (-)		1st Pod (d)		Pod wt. (kg/ha)		unit wt. grain (g)	
	Value	RAE [1]	Value	RAE	Value	RAE	Value	RAE	Value	RAE	Value	RAE	Value	RAE	Value	RAE
							Wooster, Ohio, 1988									
Observed	71	-	145	-	3,976	-	8,090	-	7.65	-	91	-	5194	0%	0.151	-
Default CSPs	87	23%	-	-	3,138	21%	8,356	3%	7.67	0%	101	11%	4490	14%	0.16	6%
Hand Calibrated CSPs	73	3%	141	3%	3,781	5%	7,892	2%	6.89	10%	90	1%	5145	1%	0.157	4%
GLUE Calibrated CSPs	72	1%	145	0%	3,893	2%	7,664	5%	6.74	12%	89	2%	5163	1%	0.161	7%
							Wooster, Ohio, 1990									
Observed	-	-	150	-	3,149	-	7,113	-	7.21	-	96	-	4915	0%	0.164	-
Default CSPs	88	-	162	8%	3,718	18%	8,387	18%	7.47	4%	104	8%	5127	4%	0.168	2%
Hand Calibrated CSPs	73	-	143	5%	3,552	13%	7,450	5%	6.82	5%	91	5%	4883	1%	0.146	11%
GLUE Calibrated CSPs	71	-	148	1%	3,713	18%	7,274	2%	6.61	8%	90	6%	4957	1%	0.156	5%
							Gainesville, Florida, 1979									
Observed	38	-	93	-	2,474	-	3,893	-	3.15	-	48	-	-	-	0.175	-
Default CSPs	40	5%	114	23%	3,570	44%	5,700	46%	3.38	7%	50	4%	4936	-	0.183	5%
Hand Calibrated CSPs	37	3%	96	3%	2,831	14%	4,303	11%	2.55	19%	48	0%	3893	-	0.156	11%
GLUE Calibrated CSPs	37	3%	99	6%	2,588	5%	3,855	1%	2.16	31%	47	2%	3416	-	0.169	3%

[1] The RAE values are the relative absolute error between field observed and model simulated variables from three different sources of CSPs.

Table 8. Comparison among cultivar-specific parameters (CSPs) of 'Williams' soybean. Default CSPs are those for "generic" MG 4 cultivar.

Source of CSPs	CSDL	PPSEN	EM-FL	FL-SD	SD-PM	LFMAX	SLAVR	SIZELF	WTPSD	SFDUR	SDPDV
Default	13.09	0.294	19.4	15.0	34.00	1.030	375.0	180.0	0.190	23.0	2.20
Hand calibrated	13.40	0.285	19.0	13.8	32.20	1.000	385.0	180.0	0.180	26.0	2.40
GLUE calibrated values	13.67	0.342	18.7	15.4	36.23	1.004	425.0	143.1	0.174	23.4	2.23
(standard deviations)	(0.384)	(0.059)	(1.206)	(1.132)	(2.209)	(0.025)	(15.60)	(13.98)	(0.008)	(1.445)	(0.21)

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