Cultivar Coefficient Estimator for the Cropping System Model Based on Time-Series Data: A Case Study for Soybean

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Highlights

- Software was developed for estimation of DSSAT CSM-CROPGRO-Soybean cultivar coefficients.
- Phenology-related coefficients were estimated based on observed phenological events.
- Growth-related cultivar coefficients were estimated based on time-series observations.
- Cultivar coefficients were optimized based on single- and multiple-experiment data sets.

Abstract. *The Decision Support System for Agrotechnology Transfer (DSSAT) is one of the most popular software solutions for predicting crop growth and yield while capturing the effects of management practices and interactions between the crop and the environment. Accurate estimation of the crop cultivar coefficients that govern in-season growth and development is critical for correct yield estimates. The manual cultivar coefficient estimation process is time-consuming and results in user-dependent, subjective optimums that are difficult to reproduce. Typically, end-of-season observations (point-based) are used for estimating dynamic in-season biomass accumulation rates. The objective of this study was to develop a time-series estimator (TSE) capable of using multiple in-season observations for estimating the coefficients that define in-season growth and biomass partitioning. Using the TSE, cultivar coefficients were estimated based on multiple in-season observations of leaf area index (LAI) and shoot, leaf, and grain dry matter weights. The cultivar coefficients were estimated from single- and multiple-treatment (seasons and locations) in-season observations. This was done for two cultivars for six management × environment combinations. Estimated multiple-treatment based cultivar coefficients were evaluated with an independent data set and compared to DSSAT standard (manual) coefficients and the cultivar coefficients estimated with the GLUE method. The average normalized root mean squared error (nRSME) for LAI and shoot, leaf, and grain weights was 26% lower for one cultivar and about the same for the other cultivar when compared to the DSSAT standard. Because GLUE uses end-of-season point-based cultivar coefficient estimation, the grain weight over time was underestimated in earlier phases and more accurate toward harvest. The TSE-estimated cultivar coefficients based on 346 in-season observations across multiple target variables and six experiments more accurately reflected in-season growth and grain weight without compromising final grain weight predictions.*

Keywords. *CROPGRO-Soybean, DSSAT, Genetic coefficients, Normalized root mean square error minimization, Time-series observations.*

A wide range of crop models have been developed for various purposes, such as yield prediction, evaluation of agricultural input management, and assessment of the long-term impacts of agricultural management practices on soil and environmental degradation (Boote et al., 2010; Ewert et al., 2015; Rötter et al., 2015; Tsuji et al., 1998). In general, these models are capable of predicting crop growth and quantifying yield-limiting factors (Hoogenboom et al., 2019a; Thorp et al., 2010) while capturing the effects of crop management (fertilizer, sowing date, sowing density, etc.) and interactions between crops and the environment (soil, weather, etc.) (Jones et al., 2003). The Decision Support System for Agrotechnology Transfer (DSSAT) is a conceptual and practical solution for capturing many important factors that affect production of more than 40 crops (Hoogenboom et al., 2019a). Within DSSAT, the Cropping System Model (CSM) CROPGRO-Legume (Boote et al., 1998) simulates crop growth and development from planting to harvest on a daily basis (carbon and nitrogen balances) throughout the vegetative and reproductive stages with different biomass and yield accumulation rates.

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The CROPGRO model simulates canopy photosynthesis on an hourly basis based on leaf-level photosynthesis parameters and simulates complete plant C and N balances, including N effects on photosynthesis, biomass accumulation, and grain growth (Boote et al., 1998). Model outputs are crop growth variables, soil water, and crop N balance on a daily basis. Various legumes can be simulated with the CROPGRO model, such as soybean (*Glycine max* L. Merr.), peanut (*Arachis hypogaea* L.), dry bean (*Phaseolus vulgaris* L.), cowpea (*Vigna unguiculata* L.), faba bean (*Vicia faba* L.), velvet bean (*Mucuna pruriens* L.), and chickpea (*Cicer aretinum* L.) (Boote et al., 2009, 2021). The ability to define specific traits (species, ecotype, and cultivar) through input files allows the use of generic algorithms for simulating the growth and development of multiple crops without modifying the crop development and growth subroutines individually.

The cultivar input files contain information for differentiating cultivars within a crop species and contain parameters important for influencing photoperiodic response, photothermal duration of specific growth stages, leaf appearance rate, seed fill duration, and composition (Hoogenboom et al., 2011, 2019a). The CROPGRO cultivar file contains 18 cultivar coefficients. These cultivar coefficients are externally defined and set up in a way to enable users to modify internally defined crop growth processes, such as defining the influence of specific cultivar parameters on crop growth and development. In general, the overall model application relies considerably on the estimation of cultivar coefficients and the reliability and accuracy of their evaluation (Seidel et al., 2018). In many cases, comprehensive experimental data sets for model evaluation are rare (Hoogenboom et al., 2012; White et al., 2013; Boote et al., 2015; Kersebaum et al., 2015).

Currently, two tools are available in DSSAT for optimization of cultivar coefficients: the genotype coefficient calculator (GENCALC) (Hunt et al., 1993) and generalized likelihood uncertainty estimation (GLUE) (He et al., 2010; Jones et al., 2011; Boote, 2019). Both tools are included in DSSAT Version 4.5 (Hoogenboom et al., 2011) and later versions (Hoogenboom et al., 2019b). Both GENCALC and GLUE use end-of-season field observations (point-based) introduced into the model through FileA for estimation of cultivar coefficients. FileA contains data that are collected only once in a season, such as yield and yield components, or are summarized during the season, such as anthesis and maturity dates and maximum leaf area index (LAI). Within GENCALC, selection of optimal cultivar coefficients is based on root mean square error (RMSE) (Jones et al., 1998). The combination of cultivar coefficients with the smallest difference between the observed and model-simulated values is taken as the optimum. Within GLUE, a Monte Carlo distribution sampling method based on a Bayesian estimation approach with a Gaussian likelihood function is used for optimizing the cultivar coefficients (He et al., 2010; Jones et al., 2011). Similar to GENCALC, only end-of-season observations for multiple target variables can be introduced into GLUE through FileA for error minimization between observed and model-simulated values. The approach optimizes all phenology-related coefficients at one time, and then all growth-related coefficients, with the strong recommendation to consider multiple treatments of the same cultivar (He et al., 2010; Jones et al., 2011; Gao et al., 2020).

However, GENCALC and GLUE cannot handle inputs of time-series observations (Buddhaboon et al., 2018). Therefore, the only option for using time-series data for the optimization of cultivar coefficients is to conduct the process manually. Calibration of models with time-series data attempts to reduce the total model prediction error by changing parameters so that the simulations match or closely resemble the observations. The goal of this study was to develop a cultivar coefficient estimator based on both time-series observations and end-of-season observations. It is expected that time-series observations (multiple in-season observations) will allow more accurate estimation of cultivar coefficients because the time-series observations are the outcome of cultivar coefficient effects on dynamically varying growth rates. By extending the list of target variables to total shoot weight, LAI, leaf weight, and other observations measured during the growing season, additional aspects of the crop model performance throughout the season can be evaluated and used for estimating cultivar coefficients, in addition to the onset of flowering and crop physiological maturity.

The specific objectives of the study were to: (1) develop a method for the estimation of phenology- and growth-related cultivar coefficients for the DSSAT CSM, and (2) evaluate an error minimization method that includes single and multiple locations and seasons of experimental in-season observations with an emphasis on multiple-treatment based coefficient estimates for establishing more robust cultivar coefficients representative of multiple locations and seasons.

Materials and Methods

Experimental Data

Experimental data for soybean conducted in different locations in the U.S. were selected for testing the TSE. The experimental data were initially collected for evaluating the impact of irrigation management and weather on the performance of soybean. The experimental files, including management practices, weather, soil characteristics, and observations of crop growth and yield, are found in DSSAT Version 4.7 (Hoogenboom et al., 2019b). Four selected irrigated treatments (table 1) of soybean cultivar Bragg were grown on an Arredondo fine sand soil with planting dates in June. Detailed information on the environmental conditions (seasonal rainfall, irrigation amounts, and mean temperatures) are shown in table 1 with the corresponding row spacing, plant populations, observed yield, and biomass (Wilkerson et al., 1983; Boote et al., 1997). Soybean cultivar Williams (four selected treatments) was grown in Ohio in 1988 (irrigated) and 1990 and in Iowa in 1988 and 1990 (table 1). Detailed environmental conditions and measured data are shown in table 1, with corresponding row spacing and plant populations.

Time-Series Estimator (TSE) for Cultivar Coefficients

The time-series estimator (TSE) for cultivar coefficients was developed as a potential DSSAT plug-in with a generic

Table 1. Cultivars and crop management experiments used for model calibration and evaluation (Wilkerson et al., 1983; Boote et al., 1997).

Soybean Cultivar	Experiment Location and Year	Treatment	Planting Date	Row Spacing (cm)	Plant Population (plants m^{-2})	Seasonal Rainfall (mm)[a]	Total Irrigation (mm)	Mean Temp.[a] (°C)	Seed Yield (kg ha^{-1})	Biomass at Maturity (kg ha^{-1})
Bragg	Gainesville 1976	Irrigated	5 May	30	12.9	776	75	26.12	3439	6848
	Gainesville 1978	Irrigated	15 June	91	29.9	534	196	27.12	3041	6068
	Gainesville 1979	Irrigated	19 June	91	47.0	695	113	26.95	2891	5781
	Gainesville 1984	Irrigated	12 June	76	31.1	469	382	26.34	3723	6689
Williams	Ohio 1988	Irrigated	1 May	19	31.1	370	557	20.61	3976	8090
	Ohio 1990	Rainfed[b]	30 April	19	41.2	581	-	19.24	3149	7113
	Iowa 1988	Rainfed[c]	11 May	70	27.2	381	-	23.26	3222	6617
	Iowa 1990	Rainfed[b]	8 May	70	19.2	776	-	21.50	3168	6674

[a] During the crop growing season, from planting to harvest.
[b] Irrigation was intended but never required.
[c] Rainfed with significant water stress.

algorithm, written in Python with an intuitive interface. The TSE requires functional experimental input files in DSSAT 4.7, such as complete crop management, weather data, soil surface, and profile data, and observations stored in a time-series file (FileT) and a summary file (FileA). It assumes that functional default files are provided for species, ecotype, and cultivar.

The TSE setup and optimization was designed in three steps (fig. 1). In step 1, the treatment (or multiple treatments) that will be used for computation of the cultivar coefficients is selected. In this step, the user can select optimization of the phenology- and growth-related cultivar coefficients separately. Phenology-related coefficients in CROPGRO-Soybean are optimized during the first round. The optimization of phenological events, such as the onset of flowering and physiological maturity, is not based on time-series observations and, as such, is easier to optimize by minimizing the difference between the simulated and observed day of onset of flowering or physiological maturity.

Optimization of growth-related cultivar coefficients is conducted using all available time-series observations throughout the season and minimizing the normalized root mean square error (nRMSE) between the simulated and observed values of total crop dry weight, grain dry weight, leaf dry weight, and LAI. Based on the selected treatment, all available in-season observations are saved in a temporary file for later comparison with the simulation outputs. The initial ranges of the selected cultivar coefficients and the associated incremental steps are defined by the user. The allowed range of the cultivar coefficients is defined by the user in a program input file, based on literature knowledge and previously determined cultivars in the desired cultivar group. The initial coefficient ranges and incremental steps are read by the program, but the user can modify the ranges and increments if necessary during the coefficient estimation procedure.

In step 2 (fig. 1), the crop model is executed for each coefficient combination. Simulations are conducted for as many coefficient combinations as were defined during the coefficient preparation in step 1. After each model run, the simulated output values are extracted from the model time-series simulation outputs and saved in a TSE output file containing both simulated and observed outputs. Finally, in step 3 (fig. 1), the TSE output file is analyzed, and the coefficient combination with the smallest average nRMSE is selected as the optimum.

Depending on the selected DSSAT version, the TSE algorithm reads all available crop models listed in the SIMULATION.CDE file located in the native DSSAT directory (fig. 2a). After selecting the desired model from the list, the TSE algorithm collects the information required for running the model and modifying the cultivar files from the DSSAT configuration file (DSSATPRO) located in the DSSAT native directory (fig. 2b).

Based on the selected model and model-specific properties shown in figure 2, the TSE algorithm lists all available cultivars in the cultivar file. For the example shown in figure 2, the TSE algorithm locates the soybean cultivar file (SBGRO047.CUL) and lists all cultivars available in the file in a list widget window (fig. 3a). After a cultivar is selected from the list, the TSE algorithm locates all experiment files available in the crop directory and lists only those experiment files (fig. 3b) that contain the selected cultivar name (e.g., cultivar Bragg in fig. 3a).

Based on the selected crop model experiment file (fig. 3b), the TSE algorithm locates this specific experiment file with related in-season observations and lists the target variables in a list widget window for selection and initialization (fig. 4a). At the same time, in a different list widget window, all cultivar coefficients available in the cultivar file are listed for optimization selection (fig. 4b). One of the options in the program is to enable access only to cultivar coefficients with predefined flags for phenology (P) or growth (G), with a separate coefficient flags file. The functionality of the TSE algorithm is not dependent on these flags, but they can be used to help users who are uncertain if a coefficient is meant for optimization of a phenological event or a growth-related variable.

The TSE algorithm was written to enable cultivar coefficient estimation of all crop models available in DSSAT, including CROPGRO and CERES-style models. A more detailed description of the TSE algorithm is available in the user guidelines available in the GitHub repository (https://github.com/memicemir/TSE).

Within the CROPGRO-Soybean cultivar file, a total of 18 coefficients are available for determining plant development and growth of different cultivar groups (Boote et al., 2003) and are listed in the list widget window shown in figure 4b. In this study, the TSE was used for estimating only eleven coefficients, listed in table 2. The selected coefficients are those that differ the most within cultivar groups, have a substantial effect on the simulated outputs, and were

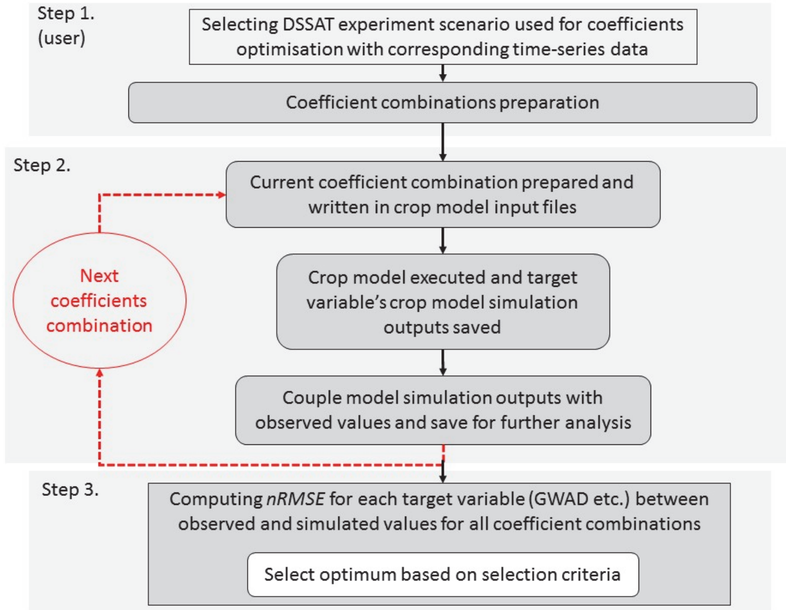
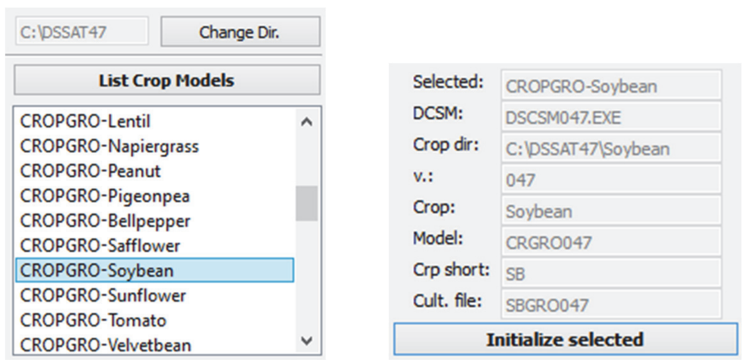
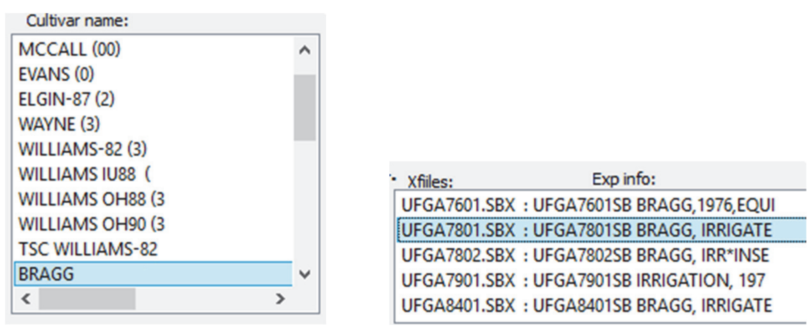


Figure 1. Flowchart of approach used for model calibration (Röll et al., 2020).



(a) **(b)**

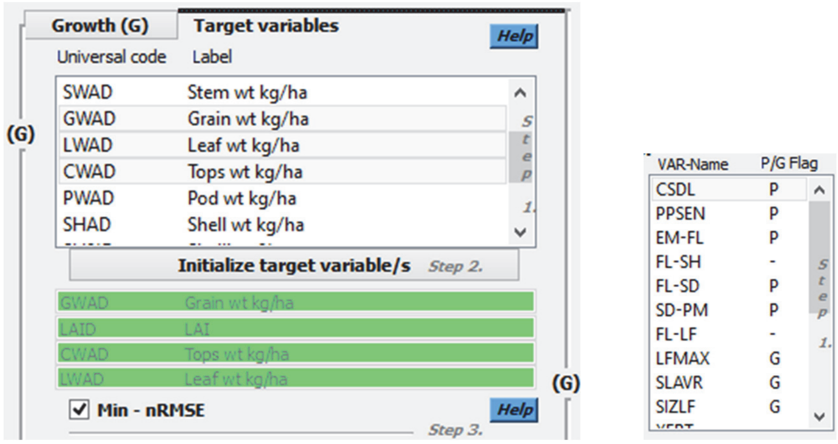
Figure 2. TSE interface for (a) list of crop models and (b) corresponding model specifications of DSSATPRO file.



(a) **(b)**

Figure 3. TSE interface for (a) cultivar list and (b) corresponding experiment files list.

designated with phenology or growth flags in figure 4b. The coefficients in table 2 are separated into coefficients used for determining the timing of cultivar-specific phenological events, such as onset of first flowering day, first pod day, first seed day, and physiological maturity day (fig. 4b, P flagged) and coefficients related to biomass and yield accumulation rates during specific growth stages (G flagged). The distinction of the coefficients into these two groups has an important theoretical and practical basis. Crop phenology depends on day length and temperature and thus is mostly independent of growth. On the other hand, crop growth (biomass and yield accumulation rates) is affected by all environmental and management factors as well as phenological development (Jones et al., 2011).



(a) (b)

Figure 4. TSE interface for (a) example for selecting growth-related target variables and (b) available cultivar coefficients.

Table 2. Coefficients targeted for optimization and their definitions in the cultivar file for CROPGRO-Soybean (Boote et al., 2003).

	Coefficient	Definition	Unit
Phenology-related coefficients	CSDL	Critical short day length below which reproductive development progresses with no day length effect (for short-day plants)	hour
	PPSEN	Slope of the relative response of development to photoperiod with time (positive for short-day plants)	1/hour
	EM-FL	Time between plant emergence and flower appearance (R1)	photothermal days
	Fl-SH	Time between first flower and first pod (R3)	photothermal days
	FL-SD	Time between first flower and first seed (R5)	photothermal days
	SD-PM	Time between first seed (R5) and physiological maturity (R7)	photothermal days
Growth-related coefficients	LFMAX	Maximum leaf photosynthesis rate at 30°C, 350 vpm CO_2, and high light	mg CO_2 m^{-2} s^{-1}
	SLAVR	Specific leaf area of cultivar under standard growth conditions	cm^2 g^{-1}
	SIZLF	Maximum size of full leaf (three leaflets)	cm^2
	WTPSD	Maximum weight per seed	g
	SFDUR	Seed filling duration for pod cohort at standard growth conditions	photothermal days

Error Minimization

Single-Treatment Normalized RMSE

For quantifying the variation between simulated (S_i) and observed (O_i) values, the nRMSE statistical method was used. The nRMSE is the RMSE (eq. 1) normalized by the mean of all available in-season observations ($\bar{O}$) for each observed crop variable, as shown in equation 2:

$$\text{RMSE} = \left[\frac{1}{n}\sum_{i=1}^{n}\left(S_i - O_i\right)^2\right]^{0.5} \quad (1)$$

$$\text{nRMSE} = \frac{\text{RMSE}}{\bar{O}} \quad (2)$$

The nRMSE is a simplified selection criterion that is applicable across multiple target variables with different scales, and because it is normalized, it can be averaged over multiple target variables. The coefficients (n coefficient combinations) are estimated across multiple target variables, with the aim of a low average nRMSE over all variables (eq. 3):

$$\text{nRMSE}_{avg(n)} = \left(\text{nRMSE}_{gwad} + \text{nRMSE}_{lai} + \text{nRMSE}_{cwad} + \text{nRMSE}_{lwad}\right) / 4 \quad (3)$$

Selection of the coefficient combination with the lowest nRMSE averaged across all target variables proved to be a good solution, as shown in table 3 for the Gainesville 1978 experiment (average nRMSE = 0.12).

Table 3. Example of varying one of the cultivar parameters (LFMAX) affecting growth-related target variables (grain weight, LAI, shoot weight, and leaf weight) for the Gainesville 1978 experiment for cultivar Bragg and selecting the optimum LFMAX value based on the lowest average nRMSE across the four target variables.

	nRMSE (unitless)				
LFMAX[a]	Grain Weight	LAI	Shoot Weight	Leaf Weight	Average nRMSE[b]
0.8	0.208	0.22	0.185	0.203	0.204
0.912	0.131	0.153	0.119	0.146	0.137
1.024	**0.082**	**0.145**	**0.109**	**0.144**	**0.12**
1.136	0.078	0.171	0.137	0.173	0.14
1.248	0.109	0.209	0.178	0.211	0.177

[a] LFMAX is defined in table 2.
[b] Average nRMSE is the average normalized RMSE over the four target variables (grain weight, LAI, shoot weight, and leaf weight).

Multiple-Treatment Goodness-of-Fit Criteria

The TSE allows users to estimate cultivar coefficients over multiple treatments. Optimization of cultivar coefficients for a single season and location is extended to optimization across multiple seasons and locations with emphasis on nRMSE values. An example of optimizing LFMAX (as defined in table 2) based on observations from three different treatments is shown in table 4. The calculated average nRMSE over the four target variables (as shown in table 3) was extended and used for determining the optimum LFMAX over multiple target variables and multiple treatments (table 4). If the number of observations is higher for

Table 4. Effect of varying LFMAX from 0.85 to 1.25 with an increment of 0.1 while determining single- and multiple-treatment optimums based on the average nRMSE for three experiments conducted in Gainesville, Florida.

Single-Treatment Optimums				Multiple-Treatment Optimums				
Year	Treatment	LFMAX[a]	Average nRMSE[b]	Year	Treatment	LFMAX[a]	Average nRMSE[b]	Multi-Treatment Average nRMSE
1978	1	0.85	0.17	1978	1	0.85	0.17	
1978	1	0.95	0.128	1979	2	0.85	0.119	0.232
1978	1	1.05	0.122	1984	3	0.85	0.408	
1978	1	1.15	0.142	1978	1	0.95	0.128	
1978	1	1.25	0.175	1979	2	0.95	0.14	0.214
1979	2	0.85	0.119	1984	3	0.95	0.374	
1979	2	0.95	0.14	1978	1	1.05	0.122	
1979	2	1.05	0.177	1979	2	1.05	0.177	0.218
1979	2	1.15	0.21	1984	3	1.05	0.355	
1979	2	1.25	0.239	1978	1	1.15	0.142	
1984	3	0.85	0.408	1979	2	1.15	0.21	0.233
1984	3	0.95	0.374	1984	3	1.15	0.346	
1984	3	1.05	0.355	1978	1	1.25	0.175	
1984	3	1.15	0.346	1979	2	1.25	0.239	0.253
1984	3	1.25	0.345	1984	3	1.25	0.345	

[a] LFMAX is defined in table 2.
[b] Average nRMSE is the average normalized RMSE over four target variables (grain weight, LAI, shoot weight, leaf weight).

one treatment than for other treatments, this procedure limits the over-representation of single-treatment effects on the multi-treatment based average nRMSE.

For each treatment, the same minimum (0.85), maximum (1.25), and increment (0.1) values for LFMAX were entered into the cultivar file (table 4). Crop model simulations were conducted for each LFMAX value, and the average nRMSE was calculated for the four target variables (grain weight, LAI, shoot weight, and leaf weight). Single-treatment optimums were available (table 4) but were ignored for calculation of the multi-treatment optimums. For each LFMAX value, a multi-treatment based average of the single-treatment nRMSE averages was calculated [(treatment 1 + treatment 2 + treatment 3) ÷ 3]. Based on the lowest multiple-treatment average nRMSE (0.214), LFMAX = 0.95 was selected as the multiple-treatment based cultivar coefficient optimum (table 4). According to the average nRMSE values shown in table 4, the optimum coefficient range for LFMAX is between 0.95 and 1.05 because those two LFMAX values had the lowest average nRMSE values of 0.214 and 0.218, respectively, when compared to the average nRMSE of other LFMAX values, such as 0.85 or 1.15. The increment could be reduced, e.g., from 0.1 to 0.01, to determine if a lower average nRMSE could be obtained with LFMAX values between 0.95 and 1.05.

Single- and Multiple-Treatment Error Minimization

The nRMSE minimization method was tested with three single treatments for estimation of the cultivar coefficients for the two soybean cultivars (Bragg and Williams), for a total of six treatments. To estimate the multiple-treatment based cultivar coefficients, three treatments were used for each cultivar. Multiple-treatment based cultivar coefficient optimums for Bragg and Williams were evaluated with data sets that were not included in the calibration process (Gainesville 1976 and Iowa 1990). The Gainesville 1976 experiment was used for evaluation because observed values for onset of flowering day, first pod, first seed, and physiological maturity were not available, and therefore optimization of phenological events was not possible. Both cultivars had been tested in the past for multiple years and different environments and had demonstrated the ability of the model to accurately simulate growth, flowering, physiological maturity, and grain yield for each cultivar in different environmental conditions (Boote et al., 1997).

The cultivar coefficients obtained with the TSE were compared with the coefficients that were distributed with DSSAT Version 4.7 (Hoogenboom et al., 2019b), which are called the DSSAT standard coefficients in this study. The cultivar coefficients that were distributed with DSSAT Version 4.7 were manually estimated by the DSSAT developers based on seven treatments for Bragg and eight treatments for Williams to obtain the best performance across multiple environments and multiple seasons per cultivar. All treatments were simulated with plant water and nitrogen balance on, and the leaf-level hedgerow photosynthesis method was selected in the corresponding experimental files. For the Iowa 1988 experiment, drought was observed, with expected stress on the observed target variables. Ideally, stress-free observations should be used for the optimization of cultivar coefficients, but one stressed treatment was included in this study to check the cultivar coefficient values estimated directly from stressed in-season observations. During the first round, the phenology-related cultivar coefficients were optimized with respect to the observed anthesis date, first pod date, first seed date, and physiological maturity. During the second round, the growth-related cultivar coefficients were estimated based on the four target variables (grain weight, leaf area index, shoot weight, and leaf weight) with in-season observations.

Because GLUE is a cultivar coefficient optimizer that is distributed with DSSAT, it was important to compare the TSE approach (time-series) to the GLUE approach (end-of-season). To enable direct comparisons of the DSSAT standard, TSE approach, and GLUE approach, GLUE was used for estimating multiple-treatment based cultivar coefficients with the same sets of three treatments. For estimating Bragg cultivar coefficients with multiple treatments with GLUE, the Gainesville 1978, Gainesville 1979, and Gainesville 1984 experiments were used. For estimating Williams cultivar coefficients, the Ohio 1988, Ohio 1990, and Iowa 1988 experiments were used. The number of simulations for the GLUE coefficient estimation process was 6000 for phenology-related target variables and 6000 for growth-related target variables.

RESULTS

SINGLE- AND MULTIPLE-TREATMENT GOODNESS-OF-FIT

The statistics for the TSE single-treatment (S-T) Bragg and Williams cultivar coefficients are shown in table 5 for phenology and in table 6 for growth. The agreement of the simulated and observed onset of flowering day, first pod day, first seed day, and physiological maturity day is shown in table 5 as the event error, i.e., the difference between simulated and observed phenological events (error = simulated – observed). The total absolute error over all simulated phenological events of Bragg cultivar for the Gainesville 1978 (S-T) experiment was 5 days and was calculated as the sum of the absolute event errors for each phenological event [|(+2)| + |(-1)| + |(0)| + |(-2)| = |5|] to prevent error compensation in the process of summation. Optimization of the phenology-related TSE Bragg coefficients resulted in an almost perfect agreement between simulated and observed phenological events for the Gainesville 1979 and 1984 (S-T) experiments, with total absolute errors of 0 and 1 day, respectively. TSE Williams optimization resulted in only 2 days total error for the Iowa 1988 (S-T) experiment and 4 days for the Ohio 1988 (S-T) experiment over the four phenological events (table 5). For the Ohio 1990 (S-T) experiment, perfect agreement was achieved between simulated and observed data for three phenological events, with the onset of flowering reported as missing.

The TSE multiple-treatment (M-T) Bragg cultivar coefficients were also used for simulating phenological events and target growth variables for the Gainesville 1978, 1979, and 1984 experiments. The corresponding statistics are shown in table 5 for phenology and in table 6 for growth. The total absolute error over all M-T simulated phenological events with TSE Bragg was 3 days for the Gainesville 1978 experiment, 6 days for the Gainesville 1979 experiment, and 2 days for the Gainesville 1984 experiment, resulting in an almost perfect agreement between the simulated and observed data. Multiple-treatment based coefficients for Williams were used for simulating phenological development

Table 5. Measures of agreement between simulated and observed phenological events as days after planting (DAP) for single-treatment (S-T) and multiple-treatment (M-T) based TSE cultivar coefficient estimates for cultivars Bragg and Williams, each evaluated over three locations.[a]

		Bragg						Williams					
		Gainesville 1978		Gainesville 1979		Gainesville 1984		Ohio 1988		Ohio 1990		Iowa 1988	
		DAP	Error	DAP	Error	DAP	Error	DAP	Error	DAP	Error	DAP	Error
S-T	Anthesis	47	(+2)	43	(0)	48	(+1)	71	(0)	76	ND	51	(0)
S-T	First pod	66	(-1)	60	(0)	66	(0)	87	(-4)	96	(0)	70	(-1)
S-T	First seed	77	(0)	69	(-)	78	(0)	100	(0)	101	(0)	83	(+1)
S-T	Maturity	114	(-2)	119	(0)	121	(0)	145	(0)	150	(0)	129	(0)
S-T	|Total error|		|5|		|0|		|1|		|4|		|0|		|2|
M-T	Anthesis	45	(0)	44	(+1)	45	(-2)	74	(+3)	73	ND	55	(+4)
M-T	First pod	65	(-2)	64	(+4)	66	(0)	91	(0)	92	(-4)	74	(+3)
M-T	First seed	77	(0)	75	ND	78	(0)	98	(-2)	101	(0)	83	(+1)
M-T	Maturity	117	(+1)	118	(-1)	122	(0)	146	(+1)	149	(-1)	128	(-1)
M-T	|Total error|		|3|		|6|		|2|		|6|		|5|		|9|

[a] Error = event error (i.e., simulated – observed), -/+ = underestimated/overestimated, and ND = no data; |Total error| = total absolute error.

Table 6. Measures of agreement between simulated and observed growth variables for single-treatment (S-T) and multiple-treatment (M-T) based TSE cultivar coefficient estimates for cultivars Bragg and Williams, each evaluated over three locations with multiple in-season observations.[a]

		Bragg						Williams					
		Gainesville 1978		Gainesville 1979		Gainesville 1984		Ohio 1988		Ohio 1990		Iowa 1988	
		RMSE	Obs.	RMSE	Obs.	RMSE	Obs.	RMSE	Obs.	RMSE	Obs.	RMSE	Obs.
S-T	Grain weight	140	7	166	8	235	7	236	17	166	18	251	10
S-T	LAI	0.41	15	0.54	17	0.39	17	0.77	17	0.96	18	0.39	9
S-T	Shoot weight	486	15	414	17	305	17	826	17	491	18	548	9
S-T	Leaf weight	143	15	179	17	99	17	305	17	253	18	207	9
M-T	Grain weight	228	7	248	8	140	7	320	17	152	18	183	10
M-T	LAI	0.47	15	0.58	17	0.51	17	0.83	17	1.02	18	0.36	9
M-T	Shoot weight	511	15	550	17	597	17	1025	17	678	18	497	9
M-T	Leaf weight	168	15	190	17	180	17	364	17	276	18	233	9
		nRMSE	Obs.	nRMSE	Obs.	nRMSE	Obs.	nRMSE	Obs.	nRMSE	Obs.	nRMSE	Obs.
S-T	Grain weight	0.07	7	0.086	8	0.114	7	0.194	17	0.163	18	0.319	10
S-T	LAI	0.145	15	0.192	17	0.13	17	0.208	17	0.303	18	0.149	9
S-T	Shoot weight	0.108	15	0.102	17	0.066	17	0.14	17	0.104	18	0.13	9
S-T	Leaf weight	0.141	15	0.186	17	0.097	17	0.229	17	0.236	18	0.187	9
S-T	Average nRMSE	0.116		0.141		0.101		0.193		0.201		0.196	
M-T	Grain weight	0.115	7	0.129	8	0.068	7	0.264	17	0.149	18	0.232	10
M-T	LAI	0.165	15	0.204	17	0.168	17	0.225	17	0.32	18	0.134	9
M-T	Shoot weight	0.114	15	0.135	17	0.129	17	0.173	17	0.144	18	0.118	9
M-T	Leaf weight	0.166	15	0.198	17	0.175	17	0.273	17	0.257	18	0.211	9
M-T	Average nRMSE	0.14		0.166		0.135		0.234		0.217		0.174	

[a] RMSE = kg ha^{-1} for grain weight, shoot weight, and leaf weight; Obs. = number of in-season observations used in cultivar coefficient estimation.

(table 5) and four target growth variables (table 6) for the Iowa 1988 and 1990 experiments and the Ohio 1988 experiment. The total absolute error over all simulated phenological events was 6 days for the Ohio 1988 experiment, 5 days for the 1990 Ohio experiment, and 9 days for the Iowa 1988 experiment, as shown in table 5.

For estimating S-T Bragg and Williams growth-related cultivar coefficients, a total of 346 in-season observations were used over six experiments, reflecting in-season growth of four target variables for each experiment. With the exception of in-season observations of grain weight, all target variables had on average more than 15 observations per season (table 6). The lowest average nRMSE with TSE single-treatment (S-T) based estimation of various Bragg and Williams coefficient combinations over the four target variables (grain weight, LAI, shoot weight, and leaf weight) ranged between 0.101 and 0.201, indicating very good results (table 6). The RMSE between simulated and observed grain weight ranged between 140 and 251 kg ha^{-1}, which was very low and an indicator of extremely good performance because the RMSE maintains the target variable unit and was calculated over multiple in-season observations. The RMSE as a measure of agreement between simulated and observed data was extremely good for all experiments, as shown in table 6, with the exceptions of shoot weight and LAI for Ohio 1988.

The lowest average nRMSE for cultivars Bragg and Williams for the various M-T growth coefficient combinations over the four target variables ranged between 0.14 and 0.234 (table 6). The RMSE of simulated and observed grain weight ranged between 140 and 320 kg ha^{-1} over six treatments for multiple in-season observations, indicating very good performance.

Comparison of DSSAT Standard, GLUE, and TSE Estimations

The TSE and GLUE multiple-treatment based estimations of the cultivar coefficients for Bragg were conducted using the Gainesville 1978, 1979, and 1984 in-season observations (table 7). For Williams, the Ohio 1988 and 1990 experiments and the Iowa 1988 experiment were used for determining TSE and GLUE multiple-treatment based cultivar coefficients (table 7). The multiple-treatment based TSE phenology- and growth-related cultivar coefficients for Bragg and Williams were similar to the DSSAT standard values (table 7), with minor exceptions for Williams for coefficients CSDL and PPSEN (phenology) and SLAVR (growth). Based on the multiple-treatment based cultivar coefficient values and comparison with the DSSAT standard Bragg and Williams values (table 7), it can be concluded that TSE was able to determine good values for the cultivar coefficients that were comparable to the values that had been determined manually by the DSSAT developers using seven or eight experimental data sets for each cultivar.

The TSE multiple-treatment based cultivar coefficients that were estimated for Bragg and Williams (table 7) were used for simulating four phenological events and four target growth variables for one independent data set for each cultivar. The multiple-treatment based TSE cultivar coefficient estimates were comparable to the DSSAT standard Bragg and Williams coefficients, indicating the potential of using TSE for estimating generic phenology-related coefficients. The 1990 Iowa experiment was used for evaluating the TSE-based Williams cultivar coefficients. In this experiment, the first pod day and first seed day were not observed. Physiological maturity simulated with the TSE Williams cultivar coefficients (table 8) was more accurate when compared to the DSSAT standard values for Williams, based on the observed data.

The TSE average nRMSE for various coefficient combinations for the four target growth variables (grain weight, LAI, shoot weight, and leaf weight) was 26% lower for the Gainesville 1976 experiment (cultivar Bragg) and the same for the Iowa 1990 experiment (cultivar Williams) as compared to the DSSAT standard Bragg and Williams cultivar coefficients (table 8). For the Gainesville simulations with the TSE multiple-treatment coefficient optimums (table 7), the RMSE and nRMSE values were lower when compared to the DSSAT standard Bragg coefficient simulations for all four target variables (table 8). For the Williams cultivar simulated for Iowa 1990, the RMSE and nRMSE values for the four target variables were similar to the DSSAT standard simulations (table 8), with minor improvement for the simulation of grain weight and worsening for the simulation of LAI.

Table 7. Multiple-treatment based TSE and GLUE phenology- and growth-related cultivar coefficient values for Bragg and Williams for three locations each and compared with DSSAT standard values.[a]

	Bragg			Williams		
Coefficients	DSSAT Standard	GLUE (Gainesville 1978, Gainesville 1979, Gainesville 1984)	TSE (Gainesville 1978, Gainesville 1979, Gainesville 1984)	DSSAT Standard	GLUE (Ohio 1988, Ohio 1990, Iowa 1988)	TSE (Ohio 1988, Ohio 1990, Iowa 1988)
Phenology coefficients defined in table 2						
CSDL	12.33	12.36	12.56	13.40	12.86	12.64
PPSEN	0.320	0.365	0.389	0.285	0.225	0.182
EM-FL	19.5	17.44	18.86	19.0	16.03	19.19
FL-SH	10.0	10.0	10.11	8.3	8.3	8.48
FL-SD	15.2	19.21	17.29	14.2	19.22	12.60
SD-PM	37.6	33.72	38.85	32.2	27.85	34.92
Growth coefficients defined in table 2						
LFMAX	1.00	1.000	0.995	0.99	1.171	1.013
SLAVR	355.0	302.6	356.0	385.0	377.9	425.3
SIZLF	170.0	187.1	162.0	180.0	228.5	166.1
WTPSD	0.17	0.170	0.219	0.18	0.189	0.199
SFDUR	25.0	17.00	23.0	26.0	18.80	26.77

[a] DSSAT standard used seven treatments for Bragg and eight treatments for Williams.

Table 8. Measures of agreement between simulated and observed phenological events as days after planting (DAP) and growth variables for DSSAT standard, GLUE, and TSE cultivar coefficients when evaluated for Bragg and Williams using an experiment that was not included in the coefficient estimation process.[a]

	Bragg (Gainesville 1976)				Williams (Iowa 1990)			
	DSSAT Standard	GLUE	TSE	Obs.	DSSAT Standard	GLUE	TSE	Obs.
Anthesis DAP	50	49	49	ND	62	57	61	66
First pod DAP	80	86	83	ND	81	79	80	ND
First seed DAP	92	106	99	ND	94	101	89	ND
Maturity DAP	143	148	147	ND	131	135	135	139
	RMSE				RMSE			
Grain weight	582	254	408	7	174	269	153	9
LAI	1.39	1.03	1.11	20	0.24	0.62	0.33	9
Shoot weight	335	621	288	20	454	1112	410	9
Leaf weight	300	251	192	20	158	408	160	9
	nRMSE				nRMSE			
Grain weight	0.368	0.161	0.258	7	0.214	0.331	0.188	9
LAI	0.422	0.312	0.337	20	0.081	0.21	0.112	9
Shoot weight	0.075	0.138	0.064	20	0.106	0.261	0.096	9
Leaf weight	0.246	0.206	0.158	20	0.161	0.414	0.162	9
Average nRMSE	0.277	0.204	0.204		0.14	0.304	0.14	

[a] Obs. = number of in-season observations used for evaluation (ND = no data); RMSE = kg ha^{-1} for grain weight, shoot weight, and leaf weight.

The GLUE multiple-treatment based Bragg and Williams cultivar coefficients (table 7) were evaluated with an independent experimental data set for Bragg (Gainesville 1976) and for Williams (Iowa 1990), similar to the TSE approach. The resulting statistics (table 8) show some important variations in the first seed and first pod dates, while the results for the onset of flowering and crop maturity were within an acceptable range for all three optimization approaches (table 8). Based on the RMSE values for the four target variables, all three optimization approaches were satisfactory, with TSE resulting in lower overall errors. With the TSE approach, additional biomass variables were included in the optimization process, such as shoot weight and leaf weight.

Time-series graphs of grain weight and shoot weight for Bragg (Gainesville 1976) and Williams (Iowa 1990) are shown in figures 5 and 6, respectively. Because GLUE uses an end-of-season point-based estimation approach for cultivar coefficients, the grain mass over time was under-estimated in earlier stages and more accurate toward harvest (figs. 5a and 6a). A higher number of optimization combinations in GLUE resulted in more accurate grain yield simulations, at the cost of accuracy for other target variables, as shown for the shoot weight simulations in figures 5b and 6b and table 8. For the DSSAT standard approach, the DSSAT developers were aware of the grain yield and shoot weight time-series observations throughout the season and tried to balance the resulting over- and under-estimations of multiple target variables throughout the season. The TSE similarly uses all in-season observations of multiple target variables in the estimation process, along with final end-of-season variables, and thus strikes a balance during the process of estimating cultivar coefficients throughout the growing season.

Discussion

Single-treatment cultivar coefficient estimation is based on observations from one treatment of a field experiment (i.e., a single season and location). With one year of in-season field observations, the cultivar coefficients can be adjusted to provide very good agreement between the simulated outputs and field observations. Ideally, the estimated cultivar coefficients for plant phenological development and growth should be applicable without any modifications across multiple locations and seasons. However, determining cultivar coefficients based on only one treatment and environment may result in field- and season-specific biases in the cultivar coefficients, resulting in under-performance of the model for different seasons for the same location or in

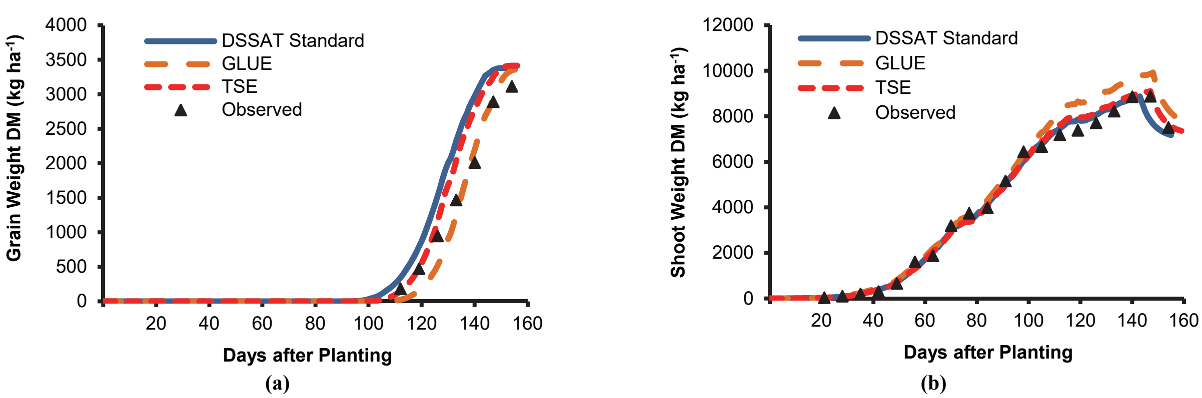


Figure 5. Time-series graphs showing simulation results for (a) grain weight and (b) shoot weight of Bragg cultivar using three optimization approaches (DSSAT standard, GLUE, and TSE). "Observed" is the Gainesville 1976 experiment data, which were not used in the cultivar coefficient estimation process.

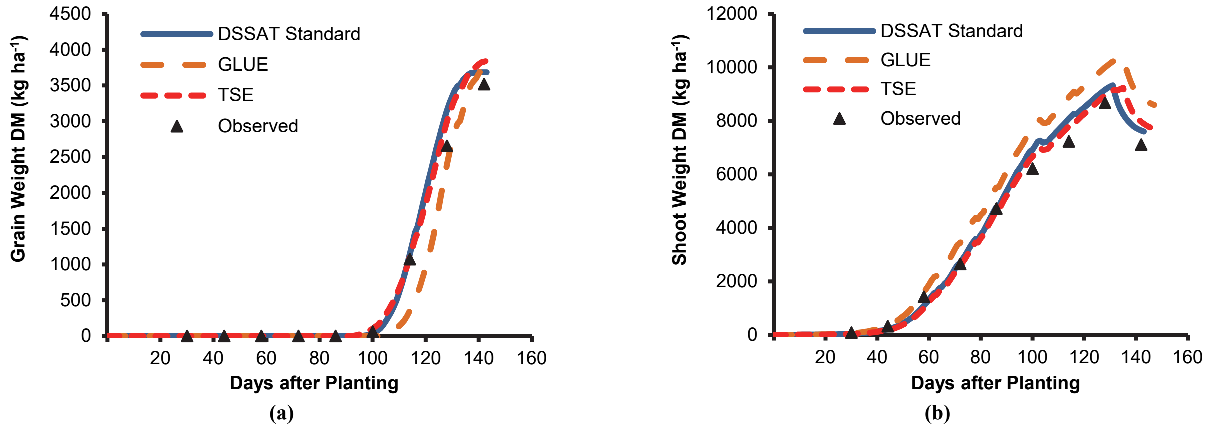


Figure 6. Time-series graphs showing simulation results for (a) grain weight and (b) shoot weight of Williams cultivar using three optimization approaches (DSSAT standard, GLUE, and TSE). "Observed" is the Iowa 1990 experiment data, which were not used in the cultivar coefficient estimation process.

other locations. Ideally, optimal (stress-free) seasonal and environmental conditions for multiple seasons and locations are required for estimating robust and representative cultivar coefficients. Because ideal conditions rarely occur in field experiments, cultivar coefficient estimation using multiple treatments, including multiple seasons and environments, is necessary to minimize the influence of season and environmental biases on cultivar coefficients.

Most of the output variables simulated with CROPGRO, such as grain yield, shoot weight, LAI, and leaf weight, do not have linear in-season growth rates. Hence, one observation at the end of the season is not sufficient for evaluation of the model results. Even if a single observation at the end of the season is perfectly simulated, that result will not provide useful insight into the dynamic growth rates that occur during the season. The influence of in-season growth rates of various variables can have an enormous influence on the above- and below-ground biomass accumulation rates, and on ratios within the above-ground biomass, e.g., stem to leaf to grain ratios. In turn, these ratios have a direct influence on the photosynthetic activity of the plants and consequently affect the end-of-season yield.

In this study, a new time-series estimator (TSE) was developed for the estimation of cultivar coefficients. The TSE provides accurate simulation of above-ground biomass and plant components based on commonly collected multiple in-season samples of four target crop variables, with emphasis on grain yield. To verify the performance of the TSE in estimating growth-related cultivar coefficients, a total 346 in-season observations of four growth variables from six field experiments were used.

The multiple-treatment based TSE coefficient optimums, shown in table 7, resulted in low average nRMSE values for the Gainesville 1978 (0.14), Gainesville 1979 (0.166), and Gainesville 1984 (1.35) experiments (table 6). As expected, the robustness of the cultivar coefficients that were estimated from more than one treatment and location resulted in less accurate single-treatment based statistics when compared to the single-treatment based cultivar coefficients for Bragg for the Gainesville 1978, 1979, and 1984 experiments, with an average nRMSE of 0.116, 0.141, and 0.101, respectively (table 6). Because single-treatment optimization allows overfitting of coefficients, the obtained results may not apply as broadly to other years and locations.

The Williams multiple-treatment coefficient optimums resulted in low average nRMSE values of 0.234, 0.217, and 0.174 for the growth variables from the Ohio 1988, Ohio 1990, and Iowa 1988 experiments, respectively (table 6). For comparison, the single-treatment based cultivar coefficients for Williams for the Ohio 1988, Ohio 1990, and Iowa 1988 experiment had average nRMSE values of 0.193, 0.201, and 0.196, respectively (table 6). Multiple-treatment based cultivar coefficient optimums that were evaluated with data not used in the coefficient estimation process showed great potential, especially when the phenology-related optimums were evaluated for Gainesville 1976. This result, along with excellent agreement of simulated and observed data for the four phenological events, allows the conclusion that the TSE performed very well in determining the cultivar coefficients.

Although any of the three coefficient optimization approaches (DSSAT standard, GLUE, and TSE) can achieve success based on the goals of a given study, there seems to be an important advantage in using multiple in-season observations across multiple target variables for estimating cultivar coefficients that correctly reflect the growth of different plant components simulated throughout entire season. The TSE allows users to select which target variables to prioritize in the coefficient optimization process, depending on the collected samples. For users who need accurate yield estimates at the end of the season, the GLUE method will likely provide accurate coefficients. For users who are investigating specific management practices with the crop model, where it is important to simulate the growth of specific plant components throughout the season (including stem to leaf to grain ratios), the TSE method is recommended to accurately evaluate the impact of those management practices.

Most important, the TSE method of cultivar coefficient optimization, based on mathematically formulated selection thresholds, eliminates user-dependent bias from the coefficient estimation process. With the removal of user bias, multi-model approaches can be implemented for specific groups of models in DSSAT, such as the three wheat models (CERES, N-Wheat, and Cropsim) and two maize models (CERES-Maize and CSM-IXIM), as described by Röll et al. (2020).

CONCLUSIONS

The TSE is designed to work with in-season field observations by minimizing the differences between simulated and observed values. Single-treatment based nRMSE error minimization showed the ability of the TSE to estimate cultivar coefficients. Based on the results of multiple-treatment based cultivar coefficient estimation, the TSE performed very well and provided robust cultivar coefficients. The TSE algorithm is written to enable optimization of cultivar coefficients for all available crop models in DSSAT. So far, it has been tested with CERES-Maize and CERES-Wheat, with satisfactory results (unpublished). It should work for many of the CROPGRO crops, especially grain legumes, because they share common cultivar coefficients and definitions. Future work will test the TSE with CROPGRO and CERES models with a focus on using time-series plus end-of-season observations, rather than only end-of-season observations, for deriving crop-specific cultivar coefficients, which is a limitation of the current GENCALC and GLUE methods in DSSAT.

The TSE software is available in the GitHub repository (https://github.com/memicemir/TSE). It can be used without any given warranty or usage restrictions. Feedback regarding TSE performance and suggestions for improvement are welcome.

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