

Simplifying the prediction of phenology with the DSSAT-CROPGRO-soybean model based on relative maturity group and determinacy



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ABSTRACT

The use of crop models can be limited by the need to calibrate cultivar coefficients across a sufficiently wide range of environments. The DSSAT-CROPGRO-Soybean crop simulation model considers different temperature and photoperiod sensitivities during different crop developmental stages and/or for different cultivars. The use of generic phenology coefficients specific for a range of maturity groups (MGs) could allow accurate predictions of main developmental stages in soybean without requiring calibration. Phenology data collected in 2012 and 2013 from an irrigated regional planting-date experiment with maturity group (MG) 3 to 6 cultivars and latitudes from 30.6 to 38.9°N, were used to calibrate cultivar coefficients across all the environments. A set of generic coefficients were generated based on relative maturity group (rMG) and plant growth habit. Predictions of main developmental stages in the subsequent growing season (2014) using generic coefficients were similar to predictions based on calibrated coefficients, with a RMSE across all cultivars <8 days. Several calibrations of cultivar coefficients were conducted testing different hypotheses of sensitivity to temperature and photoperiod in the model. Surprisingly, after the calibration, the model predicted with similar RMSEs the day of R1, first R5 seed, and R7 under the different hypothesis of model sensitivity to photoperiod and temperature. Therefore, the use of an optimization tool for calibration across several site x year x planting dates was efficient to obtain cultivar coefficients that minimized error in prediction, but did not provide meaningful insight regarding the mechanistic function of temperature and photoperiod coefficients describing phenology prediction.

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1. Introduction

1.1. Prediction of soybean phenology with mechanistic crop models

Simulation of crop phenology is essential for accurate functioning of crop models. The correct prediction of the timing of main developmental stages captures yield differences related to the length of these stages and the environmental variables that affect the crop. In soybean, this is of particular importance given the wide range of soybean maturity groups (MGs) available with different sensitivities to photoperiod and consequently variable length and timing of main developmental stages (Cregan and Hartwig, 1984). Therefore, the accurate predictions of developmental stages in soybean can have important applications for decision making and management of a range of MGs at a given latitude and/or planting date.

The main abiotic factors that have been identified as drivers of phenology in soybean are photoperiod and temperature (Cober et al., 2001; Garner and Allard, 1930; Major et al., 1975; Summerfield et al., 1998;

Wilkerson et al., 1989). The mechanism of the response to photoperiod in soybean is usually described as plants showing a maximum rate of development under short-day conditions but a slower rate of development towards reproductive stages when photoperiod is greater than a critical value (Steinberg and Garner, 1936; Summerfield et al., 1998; Summerfield et al., 1993). Within conditions of constant photoperiod, an increase in temperature was found to positively affect the rate of development, whereas it was slowed under cool or under-optimal temperatures (Garner and Allard, 1930).

To predict phenology, mechanistic crop models have been built based on hypotheses of how different phases in soybean development are distinctly affected by photoperiod and temperature. Wilkerson et al. (1989) divided the time interval from emergence to flowering in soybean into four phases that differed in their sensitivity to photoperiod: (1) a vegetative or juvenile phase that is photoperiod-insensitive, (2) a photoperiod-sensitive inductive phase, (3) a photoperiod sensitive post-inductive phase, (4) a photoperiod insensitive post-inductive phase. Alternatively, other authors have considered only three distinct phases during soybean vegetative development (Collinson et al., 1993; Ellis et al., 1992). The photoperiod-sensitive inductive phase can begin by the time the unifoliate leaves are mostly expanded, about eight days

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after sowing (Wilkerson et al., 1989), to as long as 11 to 33 days depending on the cultivar (Collinson et al., 1993). The effect of temperature and photoperiod on post-flowering development in soybean has received less attention, but there is evidence that reproductive stages after R1 are affected by photoperiod (Summerfield et al., 1998). Asumadu et al. (1998) identified a photoperiod sensitive followed by a photoperiod insensitive phase in the length of flowering time for an indeterminate MG 4 cultivar. There is less information on the effect of photoperiod on seedfill duration, but results from a simulation study concluded that both prediction of beginning seedfill and physiological maturity are more accurate when sensitivity to photoperiod is allowed to increase after flowering (Grimm et al., 1994).

Temperature is considered to positively affect the rate of development throughout the plant cycle. Experiments with soybean isolines and crop modelling studies indicate that cultivars show variable sensitivities to photoperiod but a more similar response to temperature (Grimm et al., 1994; Upadhyay et al., 1994). Other simulation studies indicate that later MG cultivars require higher temperatures than the early MG cultivars to achieve similar rates of development towards flowering (Sinclair et al., 1991). Separate temperature functions for vegetative, flowering, and beginning seedfill allowed some authors to obtain better model predictions of developmental stages (Grimm et al., 1994; Piper et al., 1996; Setiyono et al., 2007), leading them to conclude that rate of development is less sensitive to temperature in later growth stages.

A variety of crop models have developed approaches to simulate soybean phenology based on temperature and photoperiod functions that affect the rate of development during different development phases (Grimm et al., 1994; Hodges and French, 1985; Major et al., 1975; Piper et al., 1996; Setiyono et al., 2007). The complexity of a model increases as the number of developmental phases increases and as specific temperature and photoperiod functions for each phase are included. The DSSAT-CROPGRO model (Boote et al., 1998b; Hoogenboom et al., 2012; Jones et al., 2003) was selected for this study since it allows sufficient complexity and flexibility to modify temperature and photoperiod sensitivity during different stages of development. Moreover, the DSSAT model has been previously tested in soybean (Boote et al., 1997), for studying the effect of management and/or environmental conditions (Curry et al., 1995; Egli and Bruening, 1992), and it offers the feasibility to study crop rotations (Salmerón et al., 2014b). Despite a large number of crop coefficients considered in the DSSAT-CROPGRO model, only three coefficients related to photoperiod sensitivity (CSDL, PPSEN, and R1PPO), and four coefficients related to photothermal duration of life phases (EM-FL, FL-SH, FL-SD, SD-PM) are usually calibrated at the cultivar level (Boote et al., 2001).

1.2. Determination of phenology coefficients for crop models

A dataset comprising a wide range of latitudes and planting dates is usually required to obtain robust cultivar coefficients that will be stable across different environments (Grimm et al., 1993, 1994; Mavromatis et al., 2001; Piper et al., 1996). Optimization tools can aid in selecting cultivar coefficients that can optimize predictions across a wide range of environments (Archontoulis et al., 2014). DSSAT has incorporated the Generalized Likelihood Uncertainty Analysis (GLUE) tool for calibrating sets of cultivar coefficients for growth and phenology across several treatments and environments (He et al., 2010; Jones et al., 2011).

Obtaining cultivar coefficients for commercial cultivars, usually short-lived, makes difficult the calibration across a wide range of environments and, therefore, the application of crop models. There is increasing interest in approaches that allow simplification of the calibration of cultivar coefficients (Archontoulis et al., 2014; Irmak et al., 2000; Mavromatis et al., 2001; Setiyono et al., 2007). Soybean cultivars in the USA are classified as MGs from 000 to 12 based on their sensitivity to photoperiod. Relative MGs (rMGs) further divide each MG

into fractional numeric values. Predictions based on rMG provided by the seed companies could be useful because they do not require cultivar coefficients obtained for each cultivar. Setiyono et al. (2007) developed a model that predicts phenology of soybean MG 2 to 4 based on MG and stem termination growth type (determinate or indeterminate) and found that this simplification did not worsen significantly the prediction of main developmental stages (Setiyono et al., 2007; Torrión et al., 2011). Similarly, Archontoulis et al. (2014) developed a methodology for calibration of cultivar coefficients based on their MG classification and recorded dates of flowering and maturity. The DSSAT-CROPGRO model has a set of default generic coefficients for MG 00–9 soybean cultivars solved by Grimm et al. (1993, 1994) and Piper et al. (1996) from experimental data. In the current research, data from a large multi-location, irrigated, planting date and soybean MG study conducted in the US Midsouth with cultivars ranging from MG 3 to 6 was used to pursue the following goals:

- Evaluate the applicability of DSSAT-CROPGRO to predict main developmental stages in soybean grown across the Midsouth with cultivar specific coefficients vs. generic coefficients.
- To test the robustness of the phenology coefficients and the mechanistic phenology model by comparing different hypotheses of model sensitivity to photoperiod and temperature.

2. Materials and methods

2.1. Multi-location field experiments

A large planting date and soybean MG study was conducted at seven locations in 2012 and nine locations in 2013 and 2014 across the Midsouth. The locations were: Columbia, MO (38.9°N), Portageville, MO (36.4°N), Milan, TN (35.9°N), Keiser, AR (35.7°N), Verona, MS (34.2°N), Rohwer, AR (33.8°N), St. Joseph, LA (32.0°N), and College Station, TX (30.6°N). At each location there were four different planting dates every year, except at Fayetteville with one single planting date. Planting dates ranged from 21 March to 17 July across the whole study. Each year, 16 commercial soybean cultivars were used, with four cultivars within each of the following MGs 3, 4, 5 and 6 (Table 1).

Some cultivars changed from one year to the next and were replaced by a cultivar within the same MG. All MG 3 and 4 cultivars had an indeterminate growth type habit, whereas MG 5 and 6 cultivars had a determinate one (with the exception of an indeterminate MG 5 cultivar, AG5335). The experimental design used for each year and location

Table 1

Soybean cultivars within each maturity group (MG) 3 to 6 and relative maturity group (rMG) provided by the seed companies.

MG	2012		2013		2014	
	Cultivar	rMG	Cultivar	rMG	Cultivar	rMG
III	5N342R2	3.4	5N342R2	3.4	5N342R2	3.4
	RT 3644	3.6	R2 36X82N	3.6	R2 36X82N	3.6
	P93Y72	3.7	P93Y72	3.7	P39T67R	3.9
	P93Y92	3.9	P93Y92	3.9	P93Y92	3.9
IV	42-M1	4.2	42-M1	4.2	42-M1	4.2
	P94Y40	4.4	P94Y40	4.4	P46T21r	4.6
	AG4732	4.7	AG4732	4.7	AG4730	4.7
	REV49R11	4.9	REV48R33	4.8	REV48R33	4.8
V	AG5332	5.3	AG5332	5.3	AG5332	5.3
	AG5532	5.5	AG5532	5.5	AG5532	5.5
	P95Y50	5.5	P95Y50	5.5	P54T94R	5.4
	P5811RY	5.8	P5711RY	5.7	P5711RY	5.7
VI	6202-4	6.2	6202-4	6.2	AG6534	6.5
	P96M60	6.6	AG6132	6.1	AG6132	6.1
	AG6732	6.7	AG6732	6.7	AG6732	6.7
	HBKR7028	7.0	P6710RY	6.7	P6710RY	6.7

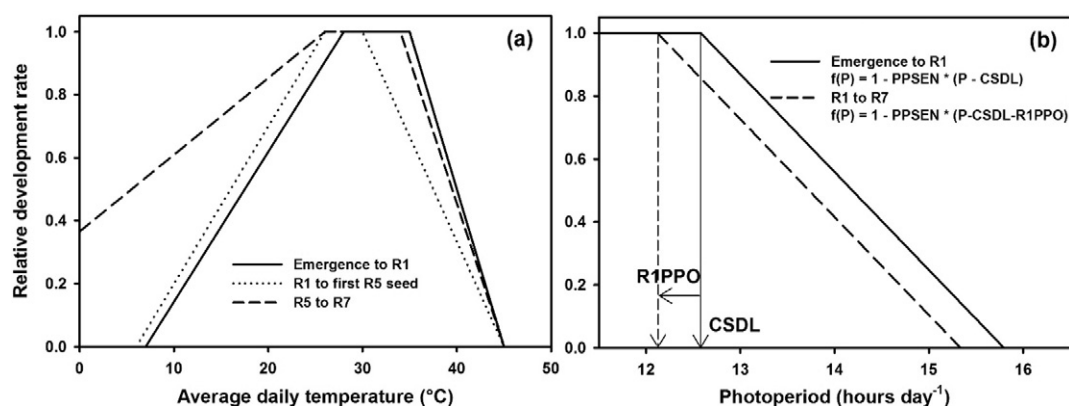


Fig. 1. Temperature functions in DSSAT-CROPGRO-Soybean for vegetative (Emergence to R1), early reproductive (R1 to first R5 seed), and late reproductive (first R5 seed to R7) stages that describe rate of development as a function of average daily temperature (a). Example photoperiod functions in DSSAT-CROPGRO-Soybean for a MG 6 cultivar for vegetative (Emergence to R1) and reproductive stages (R1 to R7) describing the rate of development as a function of daily photoperiod (h day⁻¹) (b). A critical photoperiod below which there is a maximum rate of development is indicated by the cultivar coefficient CSDL, the slope of the response to above critical photoperiod values is represented by the coefficient PPSEN, and R1PPO represents the decrease in CSDL during reproductive stages.

was a split-plot, with planting date as the whole plot factor, and cultivars nested within a MG as subplots. Plots were 6 m long and had four single or four pairs of twin rows. Row spacing was dependent on the location: 76 cm (Columbia, Portageville, and Milan), 51 cm (St Joseph), 48 cm (Fayetteville and Rohwer in 2013), 38 cm (College Station), and 19–20 cm twin rows on 97 cm beds (Keiser and Rohwer in 2013 and 2014). The most common soil textural classification across experiments was silt loam, followed by clay loam (Verona and College Station), silty clay (Keiser), and clay (St Joseph). All experiments were irrigated. Further details of the experiments can be found in Salmerón et al. (2014a and 2016).

Developmental stages at the whole canopy level were recorded from two replicates of each treatment at each year and location. The following stages were recorded according to Fehr and Caviness (1977): date of emergence (50% of plants with cotyledons), beginning flowering or R1 (first open flower on the main stem in 50% of plants), beginning seed stage or R5 (seeds of at least 3 mm in any of the four uppermost nodes in 50% of the plants), and physiological maturity or R7 (one mature pod in any node on the main stem in 50% of the plants). Additionally, the day of the first R5 seed (3 mm) at any node on the main stem in 50% or more of plants was recorded.

2.2. DSSAT-CROPGRO phenology model

The DSSAT model v. 4.5.1.023 (Hoogenboom et al., 2012; Jones et al., 2003) was used for this study. DSSAT-CROPGRO simulates soybean phenology based on 13 possible life-cycle phases from sowing to maturity (Boote et al., 1998a). There is a development rate that is a function of temperature, photoperiod, and water and nitrogen deficits. For the irrigated conditions of this study, only temperature and photoperiod effects on the crop were considered (Eq. 1), and development rate was expressed as photothermal days (PD) per calendar day.

$$PD/day = f(T) * f(P) \quad (1)$$

The temperature function in CROPGRO, $f(T)$, is different for the vegetative (emergence to beginning flowering), early reproductive (beginning flowering to first R5 seed), and late reproductive (first R5 seed to physiological maturity) stages (Fig. 1a). The photoperiod function, $f(P)$, is composed of a critical photoperiod below which the crop develops at an optimum rate (CSDL), and a decrease in development rate occurs with longer photoperiods with a slope, PPSEN (Fig. 1b). Additionally, the sensitivity to photoperiod after R1 can increase by subtracting a number of hours (R1PPO) to the critical photoperiod (CSDL) (Fig. 1b). A development phase is completed after a number of physiological

days that can be constant across cultivars or change with soybean MG and/or cultivar type. DSSAT-CROPGRO usually requires calibration for the number of physiological days from emergence to flowering (EM-FL), time between first flower and first R3 pod (FL-SH), time between first flower and first R5 seed (FL-SD), and time between first R5 seed and physiological maturity (SD-PM). Additionally, R1PPO can be calibrated at the cultivar level. The list of cultivar coefficients in DSSAT-CROPGRO related to phenology and commonly requiring cultivar specific calibration is presented in Table 2. Further details of the phenology model in DSSAT-CROPGRO are provided by Boote et al. (1998a, 1998b).

2.3. Estimation of phenology coefficients

Calibrations were performed with data from 2012 and 2013 across all locations and treatments ($n = 25$ to 58 for each cultivar). The Generalized Likelihood Uncertainty Analysis (GLUE) in DSSAT (He et al., 2010) was used to conduct calibrations. The GLUE methodology (Beven and Binley, 1992) is a Bayesian method to estimate coefficients that uses a Monte Carlo sampling from prior distributions of the coefficients. In this study, the GLUE tool was set to generate a total of 10,000 randomized sets of coefficients for each calibration. A set of cultivar coefficients is generated modifying some of the parameters related to phenology

Table 2

Generic phenology coefficients for DSSAT-CROPGRO obtained across environments in the US MidSouth for MG 3 to 6 cultivars. The phenological coefficients were generated based on relative maturity group (rMG) and plant growth habit (determinate vs. indeterminate) after calibration with data from 2012 and 2013.

MG	rMG	CSDL ^a (h)	PPSEN ^b (h ⁻¹)	R1PPO ^b (h)	EM-FL ^a (PTD)	FL-SH (PTD)	FL-SD ^a (PTD)	SD-PM ^a (PTD)
3	3.2	13.5	0.283	0.324	17.5	6.2	14.2	34.1
	3.7	13.3	0.287	0.324	17.5	6.2	14.2	34.6
4	4.2	13.2	0.291	0.369	17.5	7.3	14.2	35.1
	4.7	13.0	0.296	0.369	17.5	7.3	14.2	35.6
5	5.2	12.8	0.300	0.414	21.0	7.6	11.6	32.8
	5.7	12.7	0.304	0.414	21.0	7.6	11.6	32.8
6	6.2	12.5	0.308	0.459	21.0	8.6	11.6	32.8
	6.7	12.4	0.313	0.459	21.0	8.6	11.6	32.8

^a Coefficients estimated from this study based on rMG and/or plant growth habit (determinate vs. indeterminate). CSDL: Critical short day length below which reproductive development progresses with no daylength effect (h); EM-FL: Time between plant emergence and flower appearance (R1) (PTD); FL-SH: Time between first flower and first pod (R3); FL-SD: Time between first flower and first seed (R5); SD-PM: Time between first R5 seed and physiological maturity (R7) (PTD).

^b Coefficients solved by Grimm et al. (1993, 1994) and Piper et al. (1996). PPSEN: Slope of the relative response of development to photoperiod with time (1/h), R1PPO: Increase in daylength sensitivity after anthesis, CSDL decreases by this amount (h).

(CSDL, PPSEN, EM-FL, FL-SD, SD-PM). Thereafter, the performance of each set of cultivar coefficients is evaluated with a likelihood measure that weights the prediction of different observed variables. Finally, the GLUE tool selects the set of cultivar parameters that optimize the prediction of the three main developmental stages. Due to the computational demand required by the GLUE optimization procedure, the computation hardware at Arkansas High Performance Computer Center (AHPCC) was used for performing parallel-wise DSSAT-GLUE runs across cultivars and/or calibration approaches.

For this study, GLUE was set to calculate likelihood values from the simulated and observed date of flowering first. Preliminary calibrations of the cultivar coefficients affecting development rate towards flowering (CSDL, PPSEN, EM-FL) revealed limitations to obtaining stable coefficients for PPSEN with our dataset. Therefore, values for PPSEN were fixed to the default by MG in DSSAT (v.4.5.1.023; Grimm et al., 1993). Thereafter, the calibrated coefficients affecting prediction of beginning flowering (CSDL and EM-FL) were fixed before setting GLUE to calibrate for prediction of first R5 seed and physiological maturity (coefficients FL-SD and SD-PM). Given that the date of first R3 pod or beginning pod was not recorded, FL-SH values were estimated proportionally to the default FL-SH/FL-SD ratio (DSSAT model v. v. 4.5.1.023) as proposed by Mavromatis et al. (2001). To optimize the coefficient R1PPO that increases the sensitivity of development after R1 to photoperiod, a series of calibrations were conducted with modifications in R1PPO from 0 to 1 h in 0.05 intervals when calibrating FL-SD and SD-PM. The optimization exercise to estimate values for R1PPO revealed that, provided enough range of variation to the coefficients FL-SD and SD-PM during calibration, the model predicted with similar accuracy dates of R5 and R7 regardless of the value given to R1PPO. Therefore, default values for R1PPO by MG in DSSAT (v. 4.5.1.023) were used to obtain calibrated coefficients.

The calibration procedure allowed cultivar specific coefficients for phenology to be obtained for a total of 21 cultivars of MG 3 to 6. Differences in phenology coefficients based on rMG and/or plant growth habit (determinate vs. indeterminate) were analyzed and used to generate a set of generic coefficients that will be presented in the results section (from now on referred as “Generic” coefficients). Additionally, model predictions with the default set of coefficients by MG in DSSAT (v. 4.5.1.023) were evaluated (referred as “Cal 0”).

2.4. Sensitivity analysis of model response to temperature and photoperiod

A series of calibrations were conducted with modifications in the sensitivity of the phenology model to changes to temperature and photoperiod. After several preliminary calibrations, some hypotheses of model sensitivity to temperature and photoperiod were selected to assess the robustness of the phenology model coupled with an optimization tool for calibration: (Cal 1 or base scenario) calibration of CSDL, EM-FL, FL-SD and SD-PM as described in the previous section, with PPSEN

and R1PPO fixed by MG according to the default values in DSSAT (v. 4.5.1.023); (Cal 2) constant sensitivity to photoperiod during vegetative and reproductive stages (R1PPO = 0 h) fixed across cultivars; (Cal 3) maximum increase in sensitivity to photoperiod after flowering (R1PPO = 1 h) fixed across cultivars; (Cal 4) calibration considering no photoperiod effect after beginning seedfill (deactivation of the linear photoperiod function after first R5 seed in the species file SBGRO045·SPE); (Cal 5) increase in the time from first true leaf to the end of the juvenile phase (V1-JU in the SBGRO045·ECO ecotype file) from 0 to 5 photothermal days; and (Cal 6) reduced sensitivity of development rate to low temperatures during seedfill (minimum temperature for development decreased from −15 to −45 °C in the species file SBGRO045·SPE).

The range of variation allowed for the generation of the randomized set of cultivar coefficients (CSDL, PPSEN, EM-FL, FL-SD and SD-PM) with the GLUE optimization tool was initially set according to Boote et al. (2003). After a preliminary calibration for each calibration scenario (Cal 1 to 7), the range of variation for each cultivar coefficient was modified depending on each scenario to allow the GLUE optimization procedure to select values outside of the initial range for some of the cultivar coefficients.

2.5. Statistics for model evaluation

The different calibrations were compared in their ability to minimize the root mean square error (RMSE) in the prediction of R1, first R5 seed and R7 for each cultivar separately (Eq. 2).

$$\text{RMSE (days)} = \left(\frac{\sum_{t=1}^N (o_t - p_t)^2}{N} \right)^{1/2} \quad (2)$$

where o_t is the observed date of R1, first R5 seed, or R7 for treatment t , p_t is the predicted date for the same development stage for treatment t , and N is the number of observations for that cultivar. The model performance is presented in the paper with averaged RMSE values across cultivars within a MG.

The model was evaluated in its accuracy to predict developmental stages for an independent growing season in 2014. Model predictions were compared when using cultivar specific calibrated coefficients for phenology vs. using coefficients generated based on rMG and plant growth habit (Generic). Model evaluation was conducted for a total of 11 cultivars previously tested during 2012 and/or 2013 and for which cultivar coefficients had been determined (Table 1). Additionally, the accuracy of the model predicting developmental stages with the generated cultivar coefficients was evaluated with a set of 5 new cultivars included in 2014 and not previously used in the calibration (Table 1).

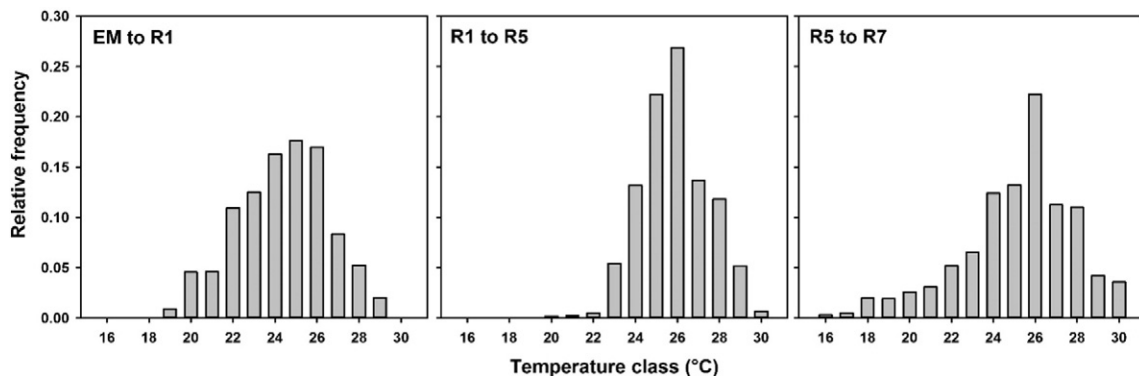


Fig. 2. Relative frequency distribution of daily average temperature during vegetative (EM–R1) (a), early reproductive (R1–R5) (b), and late reproductive (R5–R7) (c) developmental stages across all locations and years.

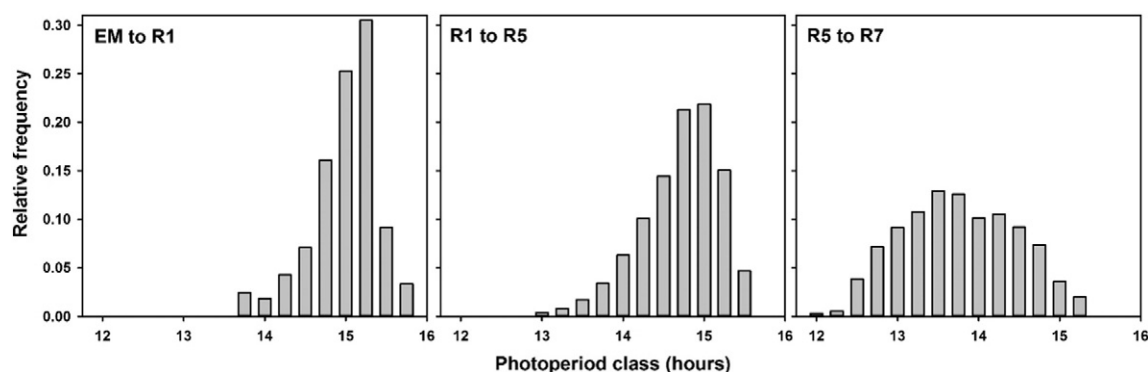


Fig. 3. Relative frequency distribution of average day length during vegetative (EM–R1) (a), early reproductive (R1–R5) (b), and late reproductive (R5–R7) (c) developmental stages across all locations and years.

3. Results

3.1. Experimental conditions and observed length of developmental stages

The relative frequency distribution of temperatures and photoperiods observed at the experimental sites, averaged across three main developmental stages (EM to R1, R1 to R5, and R5 to R7) is presented in Figs. 2 and 3. The distribution of average temperature was variable depending on the developmental stage, but in all cases included an optimum for soybean growth of 26 °C within the most frequent temperatures. It should be noted that the reported temperatures in Fig. 2 are averaged across the time interval for each developmental phase, and therefore reduce the effect of more extreme high and/or low temperatures when compared to daily values. The temperature distribution indicates that experiments were subject in most cases to under optimal and optimal temperature conditions for development, and that supra-optimal temperatures (>30–35 °C) were still present on a daily basis but to a lesser extent.

Similar to temperature, photoperiod was averaged across the time interval for each developmental stage, thereby avoiding more extreme daily values (Fig. 3). The frequency distribution indicates that in most cases, the average photoperiod for the development periods was greater than the critical photoperiod for maximum developmental rate. There was a greater frequency of short-day conditions during the late reproductive stage compared to the vegetative and flowering periods.

The average time from emergence to beginning flowering (EM–R1) across all our experimental sites increased with soybean maturity from 27.3 days in MG 3 to 51.5 days in MG 6 (Table 3). In contrast, the length from start of flowering to beginning seedfill was similar among MGs (31.2 to 34.7 days). Finally, the length of the seedfill phase increased from 35.9 in MG 3 to 41.3 days in MG 6. Therefore, differences in growth cycle across MGs were mainly associated with an increase in the length of the vegetative phase.

Surprisingly, the time interval between the first R5 seed on the main stem and beginning R5 as defined by *Fehr and Caviness (1977)* did not change substantially among cultivars with determinate growth habit

Table 3

Average number of days and standard deviation (std) for main developmental stages across all locations and years for MG 3, 4, 5 and 6 soybean cultivars.

Maturity group	Vegetative (EM–R1)		Early reproductive (R1–R5)		Late reproductive (R5–R7)		First R5 seed to beginning R5	
	Average	std	Average	std	Average	std	Average	std
3	27.3	6.0	31.2	7.7	35.9	7.1	7.5	3.6
4	30.4	6.2	33.8	8.3	39.0	7.9	8.0	4.2
5	43.2	10.6	31.7	8.7	40.4	8.5	6.9	4.1
6	51.5	11.7	34.7	10.7	41.3	9.6	6.8	4.6

(MG 5 and 6) vs. the ones with indeterminate growth habit (MG 3 and 4) (Table 3).

3.2. Calibration of cultivar coefficients with an optimization tool

An attempt to calibrate phenological coefficients using different sensitivities to photoperiod after R1 (coefficient R1PPO) produced cultivar coefficients related to photothermal duration (FL–SD and SD–PM) that had similar accuracy for predicting the date of R5 and R7 at different values of R1PPO (data not shown). Therefore, the optimization of this parameter was not possible. For this reason, R1PPO was fixed according to the values solved by *Piper et al. (1996)*. After calibration of cultivar coefficients under the base scenario (Cal 1), the RMSE in the prediction of R1 date decreased by 0.2 to 3.8 days or 2.3 days on average compared to simulations with default cultivar coefficients by MG in DSSAT (v. 4.5.1.023) (Cal 0, Table 4). The prediction of first R5 date improved to a much lesser extent, with a decrease in RMSE ranging from 0.2 to 1.6 days and 0.9 days on average. Finally, prediction of R7 date was similar after calibration (Cal 1) compared to the default phenology coefficients (Cal 0), with a decrease in RMSE ranging from –0.2 to 0.7 and 0.35 days on average. When comparing simulations by MG, predictions

Table 4

Root mean square error (RMSE) in the prediction of main developmental stages before calibration of cultivar coefficients for phenology, after different calibration hypotheses (Cal 1–Cal 6), and after generated cultivar coefficients based on rMG and plant growth habit from Cal 1.

MG	RMSE (days)							
	Cal 0†	Cal 1	Cal 2	Cal 3	Cal 4	Cal 5	Cal 6	Generic
Day of beginning flowering (R1)								
3	4.1	3.9	4.0	3.9	4.0	3.8	3.9	4.1
4	5.7	3.9	4.2	3.9	4.1	4.0	4.2	4.4
5	8.8	5.0	5.0	5.1	5.1	5.3	6.9	5.7
6	8.1	4.8	4.8	5.5	5.1	5.0	8.0	5.7
Day of first R5 seed								
3	6.6	6.4	6.7	6.5	6.6	6.2	6.8	6.6
4	9.4	7.8	8.1	7.9	8.2	7.9	8.6	8.4
5	7.3	6.1	6.5	6.0	7.1	6.4	7.4	6.6
6	6.9	6.3	6.7	6.5	7.2	6.9	8.0	7.0
Physiological maturity (R7)								
3	6.3	6.5	7.0	7.1	8.1	6.3	6.8	6.3
4	7.6	7.0	7.1	7.5	10.3	6.9	8.0	8.4
5	8.7	8.4	8.8	10.0	9.6	9.3	9.3	8.3
6	10.3	9.6	10.4	10.5	9.7	10.0	10.2	10.1

Cal 0: Cultivar coefficients by MG in DSSAT v. 4.5.1.023 obtained from *Grimm et al., (1993, 1994)*; Cal 1: R1PPO values by MG according to *Grimm et al. (1994)*; Cal 2: No increase in sensitivity to photoperiod after R1 (R1PPO = 0 h); Cal 3: same as Cal 3 but R1PPO = 1 h; Cal 4: no photoperiod effect during late reproductive stages; Cal 5: fixed increase in the length of the juvenile phase of 5 days; Cal 6: different temperature function during the late reproductive phase; Generic: cultivar coefficients based on rMG and plant growth habit derived from Cal 1.

had similar accuracy for the three main developmental stages of MG 3 cultivars after calibration compared to simulations with default coefficients in DSSAT (Cal 0) (decrease in RMSE from -0.2 to 0.2 days). For cultivars of later maturities, the prediction of R1 date improved after calibration (RMSE decreased from 1.8 to 3.8 days), followed by date of first R5 seed to a lesser extent (RMSE decreased by 0.6 to 1.6 days). On the other hand, prediction of R7 date showed little improvement after calibration (RMSE decreased from 0.3 to 0.7 days).

Overall, the model was more accurate predicting date of beginning R1 compared to date of first R5 seed, and R7 date. Moreover, calibration of cultivar coefficients did not improve the prediction of R7 date compared to using default generic coefficients in DSSAT. The RMSE expressed as a normalized value (percentage of the average observed date), were reasonably small falling below 5% for all developmental stages and MGs.

3.3. Sensitivity analysis

Successive model calibrations with the GLUE optimization tool were performed testing different hypotheses of model sensitivities to photoperiod and temperature. Cal 1 was considered as the base scenario, and the RMSE of subsequent calibrations with different hypotheses of model sensitivity to photoperiod and temperature are presented in Table 4. Calibrations were compared for their ability to minimize the RMSE in the prediction of beginning flowering (R1), beginning seedfill (first R5 seed), and physiological maturity (R7).

When considering no increase in sensitivity to photoperiod after R1 (Cal 2, R1PPO = 0 h), the calibration procedure was able to obtain cultivar coefficients that predicted main developmental stages with similar accuracy to the base scenario (Cal 1), with increases in RMSE only ranging from 0 to 0.8 days and averaging 0.3 days across MGs and developmental stages (Table 4). The contrasting scenario of an increase in 1 h of critical photoperiod after R1 (Cal 3, R1PPO = 1 h) also resulted in

simulations of similar accuracy after model calibration, with changes in RMSE ranging from -0.1 to 1.6 days and averaging 0.4 days (Table 4).

An extreme hypothesis was then tested where no photoperiod effect was considered during the late reproductive stage, and development rate during this time was solely dependent on temperature (Cal 4). The accuracy of the model predicting date of R1 and date of first R5 seed was similar to the base scenario (Cal 1) with RMSE only 0.1 to 1 day larger. The prediction of R7 date when no photoperiod function was considered was less accurate compared to the base scenario, but surprisingly only increased RMSE by 0.1 to 3.3 days and 1.6 days on average (Table 4).

Model predictions after a calibration considering an increase in the photothermal days from first true leaf to the end of the juvenile phase from 0 to 5 days (Cal 5) produced a RMSE that differed by -0.2 to 0.9 days and 0.2 days on average compared to Cal 1 (Table 4). Therefore, an increase in the length of the juvenile phase was similar to the base scenario, and overall more accurate than the other calibration hypotheses tested.

Finally, the temperature function during seedfill (first R5 seed to R7) was modified to reduce sensitivity to low temperatures during this stage by modifying the Tbase from -15° to -45°C (Cal 6). The results indicated that the model simulated date of physiological maturity with a RMSE that increased by 0 to 3.2 days and 1 day on average compared to the base scenario (Table 4).

In summary, the calibration optimization tool identified coefficients that resulted in similar RMSE in the predictions of R1, first R5 seed and R7 for models with contrasting hypotheses of sensitivity to photoperiod and temperature. Our results showed no clear evidence of model modifications to temperature and/or photoperiod response that improved model accuracy, including optimization of post flowering sensitivity to photoperiod (R1PPO). Therefore, the cultivar coefficients calibrated under the base scenario (Cal 1, Table 4) were used for generating cultivar coefficients as a function of rMG and plant growth habit, and for the subsequent model evaluation with data from the 2014 growing season.

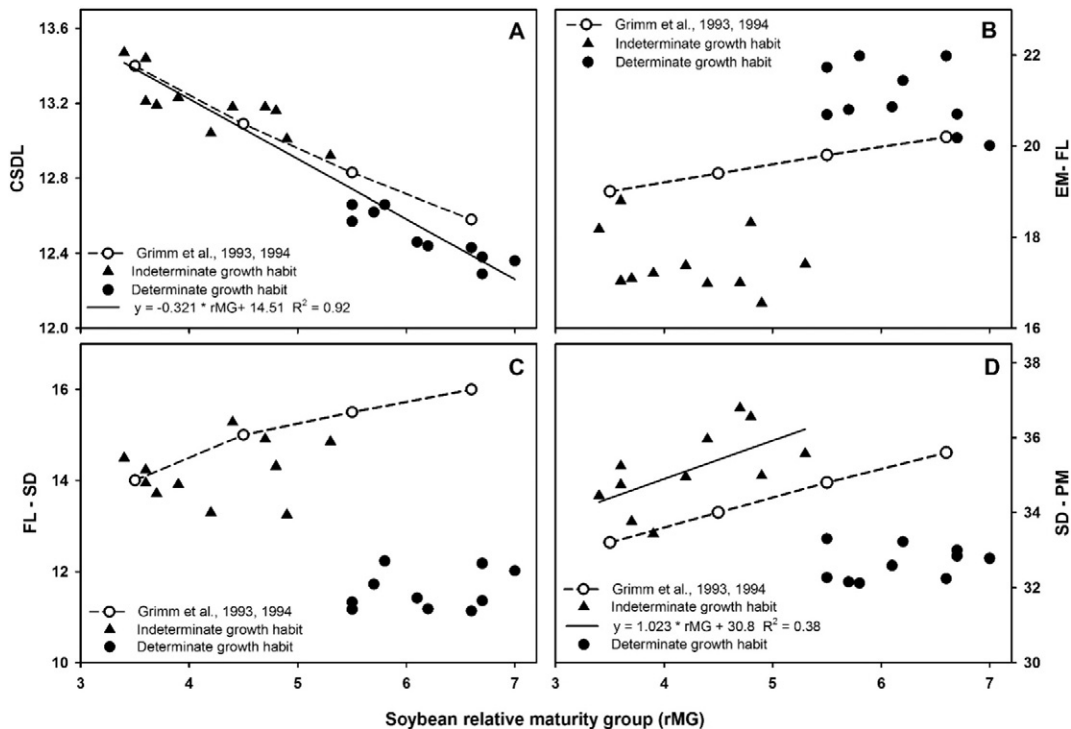


Fig. 4. Phenology coefficients in DSSAT as a function of relative maturity group (rMG) and plant growth habit (determinate vs. indeterminate): A, critical short day length (CSDL); B, photothermal days from emergence to first flower (EM-FL); C, photothermal days between first flower and first R5 seed (FL-SD); D, photothermal days between first R5 seed and physiological maturity (SD-PM). Closed symbols represent calibrated coefficients with the GLUE optimization tool under the base scenario (Cal 1), and open symbols represent coefficients by MG in DSSAT solved by Grimm et al. (1993, 1994).

3.4. Estimation of generic phenological coefficients

The values for the cultivar coefficients obtained under the calibration with the base scenario (Cal 1) are plotted as a function of rMG in Fig. 4. The results indicate that the critical photoperiod below which the plant develops at optimum rate (CSDL) decreased with maturity following a strong linear relationship ($R^2 = 0.92$) (Fig. 4A). Therefore, the rMG provided by the seed companies may allow accurate estimates for this coefficient:

$$\text{CSDL (h)} = -0.321 * \text{rMG} + 14.51 \quad (3)$$

A preliminary calibration including the slope of the decrease in development rate with photoperiod (PPSEN) showed limitations for calibrating an increasing number of coefficients. Calibrated values for PPSEN grouped close to the default values by MG in DSSAT (v. 4.5.1.023) and obtained by Grimm et al. (1993, 1994), with a bias ranging from -0.06 to 0.06 h^{-1} (data not shown). In this study, values of PPSEN were generated based on the default values by MG in DSSAT (Eq. 4). In order to fit a linear regression model, values of PPSEN from DSSAT for MG 3 to 7 were used and assigned a rMG of 3.5 to 7.5.

$$\text{PPSEN (h}^{-1}\text{)} = 0.086 * \text{rMG} + 0.255 \quad (4)$$

The photothermal days from emergence to flowering (cultivar coefficient EM-FL) were lower for cultivars with an indeterminate growth habit (2.5 photothermal days lower on average) compared to the determinate MG 5 and 6 cultivars (Fig. 4). It is interesting to note that the indeterminate cultivar within MG 5 (AG5332) obtained an optimized value for the EM-FL coefficient similar to those of other indeterminate MG 3 and 4 cultivars but different from determinate cultivars within the same MG. Following the results obtained, values for EM-FL were generated as constant values based on plant growth habit (EM-FL = 17.45 or 21.04 PTD for indeterminate and determinate cultivars, respectively).

Similarly, in the case of number of photothermal days from first flower to first R5 seed (FL-SD), there were two distinctive groups depending on the growth type habit, with indeterminate cultivars averaging 2.6 photothermal days longer on average than the determinate cultivars. Therefore, values for this coefficient were estimated as FL-SD = 14.20 or 11.57 for indeterminate and determinate cultivars, respectively. The date of first R5 seed in CROPGRO refers to the first R5 seed on the main stem, differing from the more common definition of beginning R5 by Fehr and Caviness (1977) that occurs when there is an R5 seed in any of the 4 uppermost nodes. In our study, beginning R5 occurred 7.3 days after the first R5 seed on average.

Finally, the number of photothermal days from first R5 seed to physiological maturity (SD-PM) also showed a trend related to plant growth type habit, averaging 35.12 and 32.65 days for the indeterminate and the determinate cultivars, respectively (Fig. 4). A significant linear regression ($P < 0.001$ and $R^2 = 0.38$) was obtained when plotting values of SD-PM vs. rMG for indeterminate cultivars (Fig. 4). Therefore, values for this coefficient were generated following Eq. 5 for indeterminate cultivars (SD-PM_{IN}) and for determinate ones were assigned a constant value (SD-PM_{DET} = 32.65 days).

$$\text{SD-PM}_{\text{IN}} = 1.023 * \text{rMG} + 30.805 \quad (5)$$

The number of photothermal days from flowering to beginning pod (FL-SH) was generated as function of the ratio FL-SH/FL-SD as described previously. The final set of coefficients generated based on rMG and plant growth habit for the complete list of cultivars used in our regional project is presented in Table 2. After generation of the cultivar coefficients based on rMG and growth habit, the accuracy of the model was compared to cultivar specific coefficients from Cal 1 (Generic, Table 4). The results indicated that RMSE in the prediction of developmental

stages only increased from -0.2 to 1.4 days and 0.5 days on average compared to model predictions after Cal 1.

3.5. Calibrated vs. generic phenological coefficients

The applicability of the model to predict phenological stages based on the rMG provided by the seed companies and plant growth habit was tested evaluating the model accuracy in predicting developmental stages for an independent growing season in 2014. During this growing season, 11 cultivars were part of the calibration dataset in 2012 and 2013, and five cultivars were new cultivars. Ideally, the accuracy of the model to predict phenology based on the generated cultivar coefficients would be measured with a larger number of cultivars that had not been previously used in the calibration procedure during the 2012 and/or 2013 growing seasons.

Table 5 shows the RMSE in the prediction of R1, first R5 seed and R7 in 2014 averaged by MG and comparing model predictions with cultivar specific coefficients (Cal 1) and with those generated based on rMG and plant growth habit (Generic) for the 11 cultivars that were both part of the calibration (2012 and/or 2013) and model evaluation (2014). Additionally, model predictions with generated coefficients for an independent group of cultivars ($n = 5$) is provided. The results indicate that model predictions for the set of 11 cultivars were similarly accurate when using generated coefficients based on rMG and plant growth habit compared to cultivar specific coefficients (RMSE increased from 0.2 to 0.9 days and 0.3 days on average). When testing the model accuracy with a new set of cultivars independent from model calibration, the RMSE increased from -0.5 to 3.6 days and 0.8 days on average. Overall, model predictions were as good when using cultivar specific coefficients compared to the generated ones, with a tendency for increased RMSE with late soybean maturities and later developmental stages.

4. Discussion

4.1. Calibration of phenology coefficients and sensitivity analysis

Data from this experiment included a wide range of environments ($n = 25$ to 58 site \times year \times planting dates for calibration and $n = 33$ for model evaluation), with latitudes ranging from 30.6 to 38.9°N , and planting dates from as early as late March to as late as early July. Therefore, the experimental conditions could be considered ideal for

Table 5

Root mean square error (RMSE) in the prediction of beginning flowering (R1), first R5 seed (First R5), and physiological maturity with the model evaluation dataset from 2014. The RMSE was predicted when considering phenology coefficients calibrated by cultivar during the 2012 and 2013 growing seasons (Cal 1), with estimated coefficients based on rMG and plant growth habit (Generic) from the same cultivars, and for new cultivars independent of the ones used in the calibration.

MG	RMSE (days)		
	Cal 1	Generic	Generic (new varieties 2014)
Day of beginning flowering (R1)			
3	4.7	4.8	4.9
4	4.3	4.4	4.7
5	5.2	5.7	7.1
6	5.6	6.0	8.0
Day of first R5 seed			
3	6.4	6.5	6.5
4	6.3	6.7	6.7
5	6.0	5.8	5.5
6	6.5	6.7	10.1
Physiological maturity (R7)			
3	7.1	7.5	7.5
4	6.9	7.3	7.0
5	9.4	9.9	10.3
6	11.1	12.0	10.6

calibration of phenological coefficients for a new set of cultivars for a soybean growing region compared to usually more limited site \times years and/or recorded phenological measurements (Mavromatis et al., 2001). A total of 21 cultivars were calibrated during the 2012 and/or 2013 growing seasons across the range of environments in our study. The GLUE optimization procedure allowed automatic estimation of some of the phenological coefficients in DSSAT-CROPGRO that commonly require calibration at the cultivar level (CSDL, EM-FL, FL-SD, SD-PM). The calibrated model predicted main developmental stages with a relatively low RMSE (<8 days, Cal 1).

An attempt to calibrate the coefficient R1PPO that accounts for increased photoperiod sensitivity after R1 indicated the limitations of calibrating a complex model with numerous coefficients. Conditions of equifinality in the calibration approach were evident when the optimization tool was able to generate coefficients that simulated with a similar accuracy regardless of R1PPO values. Piper et al. (1996) observed a trend for increasing sensitivity to photoperiod after R1 with later maturities (increase in R1PPO with later MGs). However, our results indicate that under the assumptions of similar increase in photoperiod sensitivity across cultivars, or even constant response of developmental rate to photoperiod during both vegetative and reproductive stages, the model predicted with similar accuracy. Therefore, conclusions regarding different photoperiod sensitivities during different developmental phases could not be drawn from our data in contrast to the results by Piper et al. (1996) with a 18° to 45° range in latitude. When Archontoulis et al. (2014) attempted to calibrate a critical photoperiod for after-flowering phases in APSIM with soybean cultivars of MG 00 to 6 and over a range of latitudes from 33 to 44°N , the authors were faced with a similar limitation, and for this reason the critical photoperiod was held constant throughout the plant cycle for each cultivar.

In DSSAT-CROPGRO, all cultivars are considered to be sensitive to photoperiod after the first true leaf (Wilkerson et al., 1989). Ellis et al. (1992) questioned the assumption that flowering response in soybean genotypes was sensitive to photoperiod soon after emergence. Moreover, Collinson et al. (1993) concluded that the time duration of the initial photoperiod-insensitive phase was a strong determinant of time of first flowering for the cultivars in their study. To test if an increase in the duration of the juvenile phase would improve predictions of developmental stages for some of the cultivars in our study, the duration of the insensitive phase was increased by five photothermal days. Our results indicated similar model accuracy after an increase in the juvenile phase of 5 days. Therefore, the simulation exercise did not identify the need for juvenile phase or potential differences in its length across the cultivars studied.

In summary, when testing contrasting hypotheses of model sensitivities to temperature and photoperiod during reproductive stages, the GLUE optimization tool was able to generate cultivar coefficients that predicted main developmental stages with a similar accuracy to the calibration under the base scenario. Therefore, the results indicate that automatic optimization tools can work successfully to obtain robust cultivar coefficients that minimize error in the prediction of developmental stages across a wide range of environments. However, our results indicate how complex crop simulation models combined with optimization tools pose limitations for testing hypotheses that can help understand and improve the processes describing development, even under a wide range of environments.

Simulation studies and coefficient optimization tools might not be sufficient to develop robust photoperiod and temperature functions, even under a wide range of environments. For instance, several modelling approaches were able to predict similarly the date of flowering in soybean (Grimm et al., 1993; Sinclair et al., 1991). More studies under controlled conditions looking at the effect of temperature and photoperiod in development to flowering and later reproductive stages are needed to further improve the processes describing phenology in crop models and allow them to include measurable differences (or coefficients) at the cultivar level. Standardized procedures to estimate critical

photoperiods and the duration of developmental stages as proposed by Ellis et al. (1992) could aid in the calibration of phenological coefficients in complex models.

4.2. Estimation of generic phenological coefficients

The analysis of the calibrated phenological coefficients for the 21 cultivars was used to generate a set of generic coefficients based on these assumptions: (i) there is a decrease in critical photoperiod (CSDL) that is related to soybean maturity, and (ii) the duration in photothermal days of some developmental stages (EM-FL, FL-SD, and SD-PM) is mainly associated with growth habit (determinate vs. indeterminate).

There was a strong relationship between the critical photoperiod below which plants develop at optimum rate (CSDL) and the soybean rMG ($R^2 = 0.92$; Fig. 4A). Piper et al. (1996) also reported a decrease in the critical short-day length with MG. Other models that use similar photoperiod functions to account for the rate of development also reported a decrease in critical photoperiod with soybean maturity (Archontoulis et al., 2014). Whereas the increase in critical photoperiod sensitivity with maturity is well reported, our results are the first to show a high agreement between this coefficient and rMG provided by seed companies for 21 cultivars of MG 3 to 6.

We found a clear effect of plant growth habit (determinate vs. indeterminate) on the duration of phases of development in photothermal days (EM-FL, FL-SD, and SD-PM). In case of photothermal time from emergence to flowering, there was an increase of 3.5 photothermal days for determinate compared to indeterminate cultivars. Our results are consistent with those reported by Piper et al. (1996) that estimated 18 and 19.5 photothermal days from emergence to flowering for MG 3 and 4 cultivars (17.5 days in our study), and 21.5 days for MG 5 and 6 cultivars (21 days in our study). Under the most inductive conditions of temperature and photoperiod in a study of near-isogenic soybean lines of the MG 4 Clark with different sensitivities to photoperiod, there were no differences in time to flowering and all lines flowered in about the same time (Cober et al., 2001). Similarly, Upadhyay et al. (1994) found no differences between isolines under most inductive conditions. These results indicate that cultivars within a plant growth type (indeterminate vs. determinate) might share a similar number of photothermal days between emergence and flowering, and that further differences in the time from emergence to flowering are mainly controlled by changes in photoperiod sensitivity.

The number of photothermal days from R1 to first R5 seed in our study was also dependent on the growth habit, decreasing by 2.4 photothermal days in determinate compared to indeterminate cultivars. Piper et al. (1996) also reported that the duration in photothermal days from R1 to R5 was larger for indeterminate cultivars compared with determinate cultivars. The authors hypothesized that the difference in photothermal days from R1 to R5 in determinate vs. indeterminate cultivars might be due to the definition of R5 by Fehr and Caviness (1977). In our study, the date of the first R5 seed on the main stem was used to calibrate the model. However, the photothermal days for indeterminate cultivars was still larger compared to determinate cultivars. Moreover, the observed date of R5 occurred at a similar time interval after first R5 seed for both determinate and indeterminate cultivars (6.8 to 8 days across MGs) when averaged across all environments.

Finally, the photothermal days from first R5 seed to R7 decreased by 1.4 to 3.1 photothermal days from the indeterminate to the determinate cultivars. There was a trend for increasing photothermal days during seedfilling with soybean maturity within the indeterminate cultivars (Fig. 4D). Overall, the prediction of the date of R7 was less accurate compared to the prediction of first R5 seed R5 and R1. Previous studies have concluded that there is more complexity in the length of photoperiod-sensitive and -insensitive periods during flowering (Asumadu et al., 1998; Upadhyay et al., 1994) than what is considered in the CROPGRO-soybean model. In the case of later reproductive stages,

there is more limited information available for the response of development rate to photoperiod and temperature.

Although it was possible to obtain calibrated generic coefficients that predicted phenology with enough accuracy and that responded to rMG and plant growth habit, the robustness and meaningfulness of these coefficients needs to be taken with caution for two main reasons. First, the sensitivity analysis indicated that the calibration optimization identified coefficients under contrasting modelling scenarios that had similar predictive ability; hence the mechanistic understanding of how these coefficients affect development should be viewed with caution. And second, limited genetic variability in commercial cultivars might explain the robustness of the generic coefficients obtained in this study; however, their applicability could be more limited when testing cultivars with a wider range of genetic variability.

4.3. Generic vs. calibrated coefficients

The need for calibrating cultivar coefficients poses limitations for the use of crop simulation models. Our results showed that when DSSAT-CROPGRO phenological coefficients were generated based on rMG and plant growth habit (determinate vs. indeterminate), the accuracy of the model was similar to calibrations that were cultivar specific, both for 11 cultivars previously used in the calibration, and for five independent new cultivars from which only rMG and plant growth habit were available.

Therefore, the simplification allowed the model to predict main developmental stages with accuracy for MG 3 to 6 cultivars grown in the Midsouth. Interestingly, simulations with default coefficients from DSSAT had similar accuracy as simulations with cultivar specific coefficients, except for the prediction of beginning flowering. Other authors were able to obtain accurate predictions with calibrations obtained by MG and plant growth habit (Setiyono et al., 2007) and with a combination of calibration settings depending on the MG and observed data for flowering and maturity (Archontoulis et al., 2014).

The set of generic coefficients for the conditions in the Midsouth solved for current cultivars and tested across a wide range of latitudes and planting dates were able to predict main developmental stages with sufficient accuracy for many agronomic purposes. The use of these generic phenological coefficients have wide applications that broaden the use of the DSSAT-CROPGRO model to study MG x planting date management strategies, rotations, and development of decision aid tools. However, even though phenological models can predict development with accuracy after calibration, improving the understanding of processes determining phenology in crop models is still necessary to broaden their applicability for breeding and genomic studies.

5. Conclusion

Simulation of soybean development with a generic set of phenological coefficients for DSSAT-CROPGRO based on rMG and plant growth habit (determinate vs. indeterminate) had similar accuracy as predictions based upon cultivar specific coefficients. The use of these generic phenological coefficients without need of calibration has wide applications to broaden the use of the DSSAT-CROPGRO model for decision tools for growers and for agronomic studies looking at potential rotations, MG and planting date treatments.

The use of the GLUE optimization tool allowed calibration of cultivar coefficients for phenology in DSSAT-CROPGRO. However, the sensitivity analysis demonstrated the limitations of the optimization procedure to resolve a meaningful and realistic set of coefficients since different sets of optimized coefficients under different scenarios of sensitivity to photoperiod and temperature gave similar accuracy. Our study indicates how optimization procedures are powerful tools for estimating cultivar coefficients across a wide range of environments, but might not improve our understanding of the processes determining phenology.

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