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A methodology and an optimization tool to calibrate phenology of short-day species included in the APSIM PLANT model: Application to soybean

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ABSTRACT

We developed a methodology and an optimization tool that simplifies calibration of the APSIM PLANT multi parameter input phenology module. The methodology and the tool were successfully applied to estimate phenological parameters for 40 soybean cultivars covering maturity groups from 00 to 6. Our approach utilized information on flowering, physiological maturity and soybean maturity group, and provided a complete set of phenological parameters for APSIM that accounted also for temperature × photoperiod interactions throughout the crop cycle. The model predicted flowering (root mean square error, RMSE = 3.1 d) and physiological maturity (RMSE = 5.5 d) very well in a range of environments across the USA (33–46°N latitude, $n = 280$). The relative absolute error was below 3% in all cases indicating the robustness of our approach. The APSIM PLANT phenology module is generic, thus our approach can be applied to all the short-day species included in the modelling platform.

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1. Introduction

Accurate simulation of crop phenology should be the first priority when calibrating simulation crop models. Phenology captures much of the genotypic variation and drives many crop-related processes in simulation models such as leaf area development, biomass production and partitioning, and also N fixation in legume species (Robertson et al., 2002). Given that phenology varies greatly among cultivars and its significant impact on crop growth simulation, phenological parameters need to be estimated every time that a new cultivar/hybrid is introduced. The lack of cultivar specific information (mainly on phenology) and the short commercial life of the cultivars impose major constrains in the application of the crop models in different locations. This is particular evident in the new era of crop model application, where multi-input parameters process-based point models are being evaluated at the regional scale (Elliott et al., 2014; Moen et al., 1994; Rosenzweig et al., 2013; van Wart et al., 2013). Setiyono et al. (2007, 2010) argued that for practical applications it is difficult to utilize a phenological model that requires numerous input parameters, especially when a minimum amount of information is available for calibration. They developed a new model for soybean that moves away from the use of multiple cultivar-specific input parameters, which are frequently not available or difficult to measure, to a more generic parameterization based on soybean maturity group (MG) and growth type (determinate and indeterminate). They also showed that this oversimplification did not impact phenology predictions significantly (Setiyono et al., 2007; Torrion et al., 2011). Other modellers have utilized the concept of the "generic cultivars" in an effort to cope with limited cultivar information (Boote et al., 2003; Yang et al., 2004).

Theoretically, an option to enhance the potential applicability of process-based models is for modellers to share cultivar information across modelling platforms. In practice, this is difficult because the phenological modules included in process-based models differ in one or more of the following aspects: phase definition, number of phases, cardinal temperature and temperature response function, photoperiod parameters and photoperiod response function, and methodology used to define phase duration (or phase targets). For example the definition and the number of phases included in the APSIM-soybean phenological module (Robertson et al., 2002; Keating et al., 2003) has many similarities with the phases defined in DSSAT-CROPGRO-soybean phenology module (Boote et al., 1998; Jones et al., 2000), it also has some similarities with

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the phases defined in SOYDEV (Setiyono et al., 2007) and it differs substantially compared to the phenological module included in the GECROS model (Yin and van Laar, 2005). On the other hand, the cardinal temperatures used, the temperature response functions and the methodology used to calculate phase "targets" in APSIM-soybean is much different compared to all the aforementioned models. Therefore, estimation of cultivar phenological parameters becomes specific for each model.

In crop models, the duration of every phase is determined by a target, which is usually expressed as thermal time target (°C-d) or number of optimum/physiological days (d). This target is modified by day-length in photoperiod sensitive species such as soybean (*Glycine max* [L.] Merr). Therefore in short or long day species the calculation of the target becomes very complex because the target varies dynamically with annual day-length fluctuations. The complexity in modelling phenology increases as the number of photoperiod sensitive phases included in the model increases. In the literature there are different methodologies to model temperature × photoperiod interactions; for an updated summary of those see Setiyono et al. (2007). Among them, the multiplicative method is widely used in many crop models such as DSSAT-CROPGRO, GECROS and SOYDEV. In this method, temperature and photoperiod functions are used as 0–1 modifiers to adjust the optimum rate of development (unit d^{-1}). A phase is completed when the accumulated daily rate of development has reached a target (e.g. 10 physiological days). Another approach is the thermal time target method (Carberry et al., 1992; Holzworth and Hammer, 1996; Carberry et al., 2001) that is used in the APSIM simulation platform. In this method, temperature is used to calculate daily thermal time (°C-d) and photoperiod to define the target as a function of day of the year. A phase is completed when the accumulated thermal time has reached the target. Though the multiplicative and the thermal time approach have conceptual differences, they both utilize the same input parameters (T_o, T_b, T_m, P_{crit}, P_{sen}, a_j; see Table 1 for acronyms definitions). The link between the two methods is illustrated in Fig. 1.

Irrespective of the methodology used, to develop parameters for a photoperiod sensitive phase multiple data points are needed. These data can be derived from field experiments with different sowing dates, years and locations or sophisticated greenhouse experiments (Grimm et al., 1993, 1994; Yin et al., 1997). It is possible to estimate phenological parameters from a single season observations by ignoring the photoperiod effect (Mohanty et al., 2012) but in this case the potential applicability of the crop model is limited.

An alternative approach for calibrating phenological parameters of photoperiod-sensitive species is to adapt optimization algorithms specifically for phenological parameters. Inclusion of optimization tools along with initial parameter values (i.e. generic coefficients) into the structure of a crop model is a very desirable feature. Such an example is the GENCALC (Hunt et al., 1993) or the more recent GLUE optimization program (Jones et al., 2011) that is included in the release of the DSSAT models (Hoogenboom et al., 2012). These tools allow DSSAT users to calibrate phenological parameters (and a few other crop parameters) of photoperiod-sensitive plants from few observations. DEVEL2 is another generic optimization program (Holzworth and Hammer, 1996) with many applications relevant to the APSIM model (Birch et al., 1998; Soltani et al., 2006). The NAG (1983) is a dedicated optimizer that has been used to estimate phenological parameters for APSIM crops (Carberry et al., 2001; Turpin et al., 2003; Farre et al., 2004). To our knowledge, these tools have not been operationally available to APSIM users and neither were they designed to optimize phenological parameters for species having sensitivity to photoperiod in both pre- and post-flowering phases. For example, Turpin et al. (2003) added functions into the NAG optimizer to estimate post-flowering photoperiodic parameters for faba bean. We believe that development of an optimization tool for APSIM to simplify phenology calibration would be advantageous for everyone working with the model, especially for those dealing with new cultivars that are responsive to photoperiod.

Table 1
List of parameters and acronyms used in this study, with their definitions, values and units. $F(t)$ indicates that the duration of a crop phase is a function of temperature. $F(p)$ indicates that the duration of a phase is a function of photoperiod.

Parameter or acronym	Definition	Value or range	Unit
MG	Soybean maturity groups	00–VI	–
DAS	Days after sowing	–	d
SOW_VE	Sowing to emergence phase	Fixed	d or °C-d
VE_JUV	Emergence to end of juvenile phase	$F(t)$	d or °C-d
JUV_FI	End of juvenile to floral initiation phase	$F(t)$ and $F(p)$	d or °C-d
FI_FL	Floral initiation to flowering phase	$F(t)$ and $F(p)$	d or °C-d
FL_SD	Flowering to start seed filling phase	$F(t)$ and $F(p)$	d or °C-d
SD_END	Start to end of seed filling phase	$F(t)$ and $F(p)$	d or °C-d
END_PM	End seed filling to phenological maturity	$F(t)$	d or °C-d
T_b	Base temperature below which the development rate is zero	10[a]	°C
T_o	Optimum temperature for maximum development rate	30	°C
T_m	Maximum temperature above which the development rate is zero	40	°C
sun_angle	Civil twilight	0	Degrees
P	Photoperiod (the length of the daylight)	0–24	Hours
P_{crit}[b]	Daylength above which the rate of development is sensitive to P	12.5–14.3	Hours
P_{crit1}	P_{crit} for pre-flowering phases (JUV_FI and FI_FL)	12.5–14.3	Hours
P_{crit2}	P_{crit} for post-flowering phases (FL_SD and SD_END)	12.5–14.3	Hours
P_{sen}[c]	Photoperiodic sensitivity coefficient	0.15–0.31	1/hours
P_{sen1}	P_{sen} for pre-flowering phases (JUV_FI and FI_FL)	0.15–0.31	1/hours
P_{sen2}	P_{sen} for post-flowering phases (FL_SD and SD_END)	0.15–0.31	1/hours
a_1[d]	Optimum or physiological days to complete VE_JUV	5	d
a_2	Optimum or physiological days to complete JUV_FI	5	d
a_3	Optimum or physiological days to complete FI_FL	1–15	d
a_4	Optimum or physiological days to complete FL_SD	9–17	d
a_5	Optimum or physiological days to complete SD_END	19–35	d
a_6	Optimum or physiological days to complete END_PM	1	d

[a] APSIM-soybean default values.
[b] Use of the P_{crit} parameter assumes $P_{crit} = P_{crit1} = P_{crit2}$. Values for P_{crit} were taken from Boote et al. (2003).
[c] Use of the P_{sen} parameter assumes $P_{sen} = P_{sen1} = P_{sen2}$. Values for P_{sen} were taken from Boote et al. (2003).
[d] An optimum or physiological day is defined as a calendar day in which temperature equals T_o and $P < P_{crit}$. By multiplying the "a_j" parameter with the term (T_o–T_b), a phase target is converted from d to °C-d.

The phenology module of the APSIM generic PLANT model provides a very flexible way to specify phenological parameters for each phase separately. Instead of using a fixed equation (i.e. linear, exponential) for the photoperiod sensitive phases, it allows the user to specify "x/y pairs" and the model reads the derived relationship by linear interpolation between the points (Holzworth and Huth, 2009). The user can input up to five X-values (photoperiod) and five Y-values (cumulative thermal time) and therefore it can produce a variety of relationships between photoperiod and

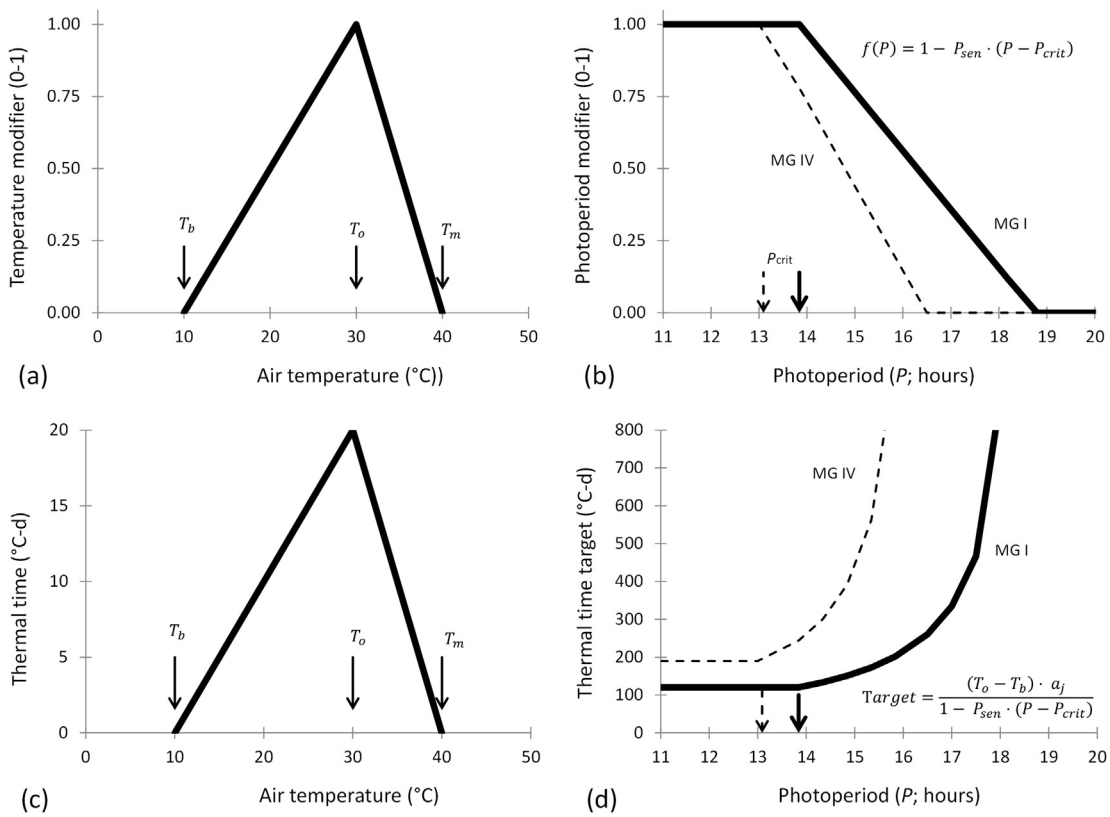

Fig. 1. Top panels: example shapes for temperature (panel a) and photoperiod (panel b) modifiers used by the multiplicative model: Rate = Rate_max · $f(T)$ · $f(P)$ in d^{-1} (see symbols explanations in Table 1). Bottom panels: temperature (panel c) and photoperiod (panel d) functions used by the thermal time target method. The two lines in panel (b) show that the photoperiod modifiers in soybean are strongly affected by maturity group. In this example, the lines were produced by using P_{sen} and P_{crit} coefficients from Boote et al. (2003) for maturity groups I and IV, respectively. P_{sen} is the photoperiodic sensitivity (slope of the line; panel b) and P_{crit} is the critical photoperiod (vertical arrows; panel c). The panel (d) is analogous to panel (b), but it reports actual thermal time values (the targets) instead of 0–1 fraction values. The term a_j refers to the number of optimum days (=calendar day in which the air temperature equals T_o and the actual photoperiod is below P_{crit}).

thermal time. This functionality allowed the APSIM team to utilize the same phenological module for the majority of the species belonging to the generic PLANT model (wheat, soybean, peanut, alfalfa, lupin, canola, chickpea, cowpea, faba bean, etc.; Wang et al., 2002; Robertson et al., 2002; Keating et al., 2003). The drawback of this method is that it is difficult to calibrate phenological parameters for new cultivars when only few observations are available. The reason is that several combinations of "*x*/*y* pairs" can provide the same result (equifinality), while the prediction ability and the behaviour of the phenological model in different environments is highly uncertain. The difficulty increases when information on calibrated cultivars in the model database is limited. For example, the APSIM-soybean model (version 7.5) contains few cultivars in the database, which do not include photoperiod effect in post-flowering phenology, even though it is known that such an effect exists (Grimm et al., 1994; Setiyono et al., 2007). This feature makes calibration of new soybean cultivars difficult and in general constrains the applicability of the APSIM soybean model in areas in which soybean is an important commodity, such as the U.S. Corn Belt region which accounts for 75% of US soybean production and 30% of global soybean production (Setiyono et al., 2010 and references therein). In general, APSIM-soybean was chosen for two reasons: a) the model attempts to chart a middle course between two types of models, a simple one (Sinclair, 1986) and a very detailed one (CROPGRO-soybean; Boote et al., 1998), so that crop growth and development can be simulated with satisfactory comprehensiveness, without the necessity of defining a large number of parameters (Robertson et al., 2002); b) belongs to a cropping systems simulation platform, which allows investigation of complex systems questions such as crop rotation (Keating et al., 2003) which cannot be investigated from stand-alone crop models.

The overall goal of this study is to expand the potential applicability of the APSIM-soybean model by developing new cultivars that cover a wide range of environmental conditions (33°–46°N latitude). More specifically, our first objective is to present and analyse a new methodology and an optimization tool that allows APSIM researchers to calibrate soybean phenological parameters from available information on flowering, physiological maturity and soybean maturity group number. The second objective is to make use of this tool (methodology and optimizer) and to produce phenological parameters for 40 different soybean cultivars covering a range of maturity groups (00–VI). The final objective is to evaluate the performance of the calibrated APSIM-soybean phenology module by conducting sensibility tests, i.e. investigate soybean adaptability in the USA and compare model predictions against soybean adaptability maps available in the literature (Zhang et al., 2007; Pedersen, 2009). Soybean is a representative of the short day species included in the generic PLANT model. This means that our approach can be applied to all the short day species and especially legume species included in the APSIM crop database.

2. Materials and methods

2.1. The APSIM model

APSIM (Agricultural Production Systems sIMulator) is an agricultural systems model that incorporates many crop and soil models into its structure and it is used worldwide to address various cropping systems aspects (Keating et al., 2003). The

majority of the crop models are structured around a generic PLANT model (Wang et al., 2002), in which crops share many functional relationships that determine plant growth and development. A full description of all APSIM's modules can be found at www.aspim.info. Herein we describe the generic PLANT phenology module with emphasis on soybean.

2.2. The phenology module

The generic PLANT phenology model can be summarized by the following equation:

$$\text{Crop cycle} = \text{SOW_VE} + \text{VE_JUV} + \text{JUV_FI} + \text{FI_FL} + \text{FL_SD} + \text{SD_END} + \text{END_PM} \quad (1)$$

where:

$$\text{VE_JUV} = (T_o - T_b)a_1$$

$$\text{JUV_FI} = \frac{(T_o - T_b)a_2}{1 - P_{\text{sen1}}(P - P_{\text{crit1}})}$$

$$\text{FI_FL} = \frac{(T_o - T_b)a_3}{1 - P_{\text{sen1}}(P - P_{\text{crit1}})}$$

$$\text{FL_SD} = \frac{(T_o - T_b)a_4}{1 - P_{\text{sen2}}(P - P_{\text{crit2}})}$$

$$\text{SD_END} = \frac{(T_o - T_b)a_5}{1 - P_{\text{sen2}}(P - P_{\text{crit2}})}$$

$$\text{END_PM} = (T_o - T_b)a_6$$

The corresponding symbol explanations are provided in Table 1. The generic PLANT phenology model utilizes the thermal time method to define phase targets (Fig. 1c and d). The targets are described in terms of thermal time requirement (phases: SOW_VE, VE_JUV, END_PM) or thermal time requirement modified by photoperiod (phases: JUV_FI, FI_FL, FL_SD, SD_END).

The SOW_VE phase is subdivided into two sub-phases: sowing to germination and germination to emergence. The duration of this phase is determined by sowing depth, air temperature, soil moisture and a number of seed–related parameters (Keating et al., 2003). Because prediction of this phase requires inputs on soil water and use of a water balance model as well, we fixed this phase from inputs on sowing and emergence dates.

The VE_JUV phase is driven by temperature and is defined as the period of development in which the rate of development is not influenced by photoperiod. Therefore, the thermal time target is a constant value (Table 1). For soybean plants, the end of juvenile phase is around the V1 stage (Wilkerson et al., 1989) according to the coding system of Fehr and Caviness (1977).

The phase JUV_FI is determined by temperature and photoperiod and ends at floral initiation. The phase FI_FL is affected by temperature and photoperiod and it is completed when 50% of the plants have one flower at any node (equivalent to R1 stage; Fehr and Caviness, 1977). The thermal time target varies dynamically with annual day-length fluctuations (Fig. 1d; Table 1). The phases FL_SD and SD_END are determined by temperature and photoperiod and refer to the period from flowering to the start of grain fill and from start to the end of the grain fill period, respectively. For the pre-flowering phases (JUV_FI and FI_FL) and post-flowering phases (FL_SD and SD_END) we used different critical photoperiod (P_{crit1} and P_{crit2}; Table 1) and photoperiod sensitivities (P_{sen1} and P_{sen2}; Table 1) parameters to add flexibility in the model and to be consistent with literature findings on soybean phenology (Grimm et al., 1993, 1994; Setiyono et al., 2007). In case of no available information, pre- and post-flowering photoperiodic parameters can be assumed the same.

The phase END_PM is determined by temperature and it is completed when 50% of the plants have reached physiological maturity (equivalent to R7; Fehr and Caviness, 1977). In APSIM there is one more phase that is not listed in Eq (1). It is the phase from physiological maturity to harvest ripe, which is not relevant in our study.

2.3. Methodology to estimate phenological parameters

We propose use of the Eq. (1) to estimate phenological parameters for soybean and more generally for the short day species included in APSIM that are included in the generic PLANT model. Eq. (1) is a compound non-linear equation with biologically meaningful parameters (Table 1). Therefore, some of the parameters can be optimized by using appropriate statistical techniques, well defined starting values and adequate datasets. Our approach to developing phenology parameters for soybean cultivars is summarized in the following steps: (1) compiled a database with soybean phenological information from the literature (Table 2); (2) utilized photoperiodic parameters from the literature (Boote et al., 2003), conducted a sensitivity analysis to identify critical parameters for optimization and developed starting values (Table 3); (3) implemented the generic PLANT phenology module into the R package; (4) selected an appropriate parameter estimation algorithm and optimized some parameters and (5) converted parameters to APSIM format, created new (phenology driven) cultivars, incorporated them into the APSIM-soybean model and tested them against the experimental data. In the future, steps 4 and 5 can be coupled.

2.3.1. Databases with phenological and weather data

Table 2 illustrates the datasets used in this study ($n = 280$). The data cover a wide range of maturity groups (from 00 to 6) and experimental sites across the USA (from 33° to 44°N). Information on sowing, emergence, flowering and physiological maturity were extracted from figures or taken from tables. When the emergence day was not provided, then simulated emergence day from the APSIM model was used. Weather data for each site were extracted from "daymet" using the reported coordinates (http://daymet.ornl.gov/) (Thornton et al., 2012). Daymet is a collection of algorithms and computer software designed to interpolate and extrapolate weather data from ground-based meteorological stations to produce gridded estimates of daily weather parameters at 1 km × 1 km resolution. The raw data (maximum and minimum temperature, precipitation, and radiation) were converted to the APSIM format (.met) using an excel-macro converter (Iowa State University; the converter is available upon request). Photoperiod is calculated by APSIM as a function of latitude, day of the year, and twilight (sun angle) (Keating et al., 2003).

2.3.2. Soybean initial parameters, sensitivity analysis and assumptions

Eq. (1) has several input parameters (Table 1). Parameters defining cardinal temperatures (Table 1) and the shape of the temperature response function (Fig. 1c) were kept similar to APSIM-soybean. Parameters describing photoperiod effects, P_{crit} and P_{sen} for each maturity group (Table 3), were taken from Boote et al. (2003). Note that these parameters were derived from a re-analysis of the detailed work done by Grimm et al. (1993, 1994) on soybean phenology. Parameters a_1 to a_6 (Table 1) were initially taken from Boote et al. (2003), but re-analysed to fit APSIM-phenological phases and re-calibrated manually to get more representative starting values (Table 3). The reason for this preliminary calibration was the large difference that existed between the temperature response functions used by APSIM-soybean and by DSSAT-CROPGRO-soybean (Jones et al., 2000). The preliminary calibration of the a_1 to a_6 parameters resulted in lower initial values.

We conducted a sensitivity analysis to identify the most critical parameters for estimation. Among the parameters included in Eq. (1) we initially prioritized for optimization the following: a_3, $[a_4 + a_5]$, P_{crit} and P_{sen} (Table 1), and assumed equal P_{crit} and P_{sen} values for pre- and post-flowering phases, $a_1 = 5$ d, $a_2 = 5$ d and $a_6 = 1$ d (Table 1; see discussion section) in order to get a reasonable number of parameters to be estimated through optimization. Ideally, it would desirable to get estimates for all the coefficients but this is constrained by limitations in statistical approaches and lack of adequate datasets.

2.3.3. The optimization program

The R software (R Development Core Team, 2005) is widely used in agronomic research to optimize parameters. We incorporated the necessary functions into R so that it was possible to replicate APSIM soybean phenology predictions to a high degree of agreement (Fig. 2). The developed R phenology program calculates:

a) daily photoperiod as a function of day of the year, latitude and solar angle;
b) daily thermal time using the 3-h interpolation method and pre-specified temperature/thermal-time relationships (Fig. 1c). We have also added more temperature/thermal-time functions which have different shapes, to allow the investigation of variable responses (Fig. S1 in the supplementary materials)
c) ASPIM's phenological stages as described in Eq. (1).

Briefly, the R optimization program works as follows. Firstly, it defines the phase targets as a function of daily photoperiod for the JUV_FI, FI_FL, FL_SD, and SD_END phases, and reads constant values for the SOW_VE, VE_JUV, and END_PM phases. The photoperiod driven targets are calculated from the equation presented in Fig. 1d. Secondly, starting at sowing, it calculates and accumulates thermal time until a target has been reached, which signals the end of a phase. Then the same process is repeated in the next phase until physiological maturity has been reached. Thirdly, it counts the number of calendar days needed to complete each phase, and outputs this information as DAS (days after sowing). Finally, it optimizes the desirable parameters by minimizing the differences between predicted and measured values using a stochastic method (see below).

The derived parameters from the optimization program were converted into APSIM format, "x/y pairs", using the following set of equations:

$$X = P_{\text{crit}} + f/P_{\text{sen}} \quad (2)$$

$$Y = a_j(T_o - T_b)/(1 - f) \quad (3)$$

where $f = 0$, 0.25, 0.50 and 0.75 (weighing factor to generate four "x/y" values); P_{crit} = critical photoperiod; P_{sen} = photoperiodic sensitivity; T_o = optimum temperature; T_b = base temperature; a_i = optimum days and it can be a_2 or a_3 or a_4 or a_5 (see Table 1 for details).

Table 2
Details of the published studies used in this analysis.

References	Years	Location	Latitude (°N)	Maturity group	# cultivars	# data[a]	Phenological data[b]	Set number
Hoogenboom et al., 2012 (DSSAT – Database)	1979 1988 1997	Iowa	42.0	2.7–3.9	5	9	VE, FL, SD, PM	1
Edwards and Purcell, 2005	2001 2002 2003	Arkansas	36.1	00–6	8	24	VE, FL, PM	2
Robinson et al., 2009	2006 2007	Indiana	40.5	2.6–3.7	3	36	VE, FL, PM	3
Setiyono et al., 2007	2004 2005	Nebraska	40.8	0.8–4.4	10	43	VE, FL, PM	4
Zhang et al., 2004[c]	2000	Mississippi	33.1	3.4–5.9	6	129	VE, FL, PM	5
Bastidas et al., 2008	2003 2004	Nebraska	40.8	3.5	1	8	FL, PM	6
De Bruin et al., 2010	2007 2009	Iowa	42.0	2	1	10	VE, FL	7
Osborne and Riedell, 2006	2002 2003 2004	S. Dakota	44.3	1	1	3	FL	8
Fermaha et al., 2012	2008 2009	Illinois	40.1	2.8–3.4	2	2	FL	9
Heatherly and Smith, 2004	2002 2003	Mississippi	33.4	4–5	2	16	FL	10

[a] Refers to the number of environments: combination of sowing time × year × location × cultivar for each study.
[b] VE: emergence; FL: flowering; SD: start of the seed fill; PM: physiological maturity.
[c] The reported data were average values across 4 experimental years for a number of cultivars.

The R code reads maximum and minimum temperature values from a csv file and days of phenological observations from a second csv file. We provide example files in the Supplementary materials (Tables S1 and S2). Within the code we have incorporated starting values for different soybean maturity groups (Table 3).

2.3.4. The parameter estimation procedure

Preliminary optimization attempts and analysis of the objective function revealed that the use of standard optimization algorithms (e.g. 'Nelder-Mead') was not appropriate due to the non-smooth objective function which resulted in most cases in a missing Hessian matrix (i.e. it could not be computed). Therefore, we developed a custom Markov chain Monte Carlo algorithm (MCMC; Givens and Hoeting, 2005). We chose this approach for two reasons: it is more robust than the optimization algorithm and it allows for a more flexible estimation of the posterior distribution of the parameters given the data. This works by generating values from proposal distributions and accepting or rejecting values depending on whether they generate values consistent with a distribution of the parameters given the data (Givens and Hoeting, 2005). From these distributions we estimated the parameters for the soybean model from the median of the posterior distribution. The algorithm produces candidate values for the parameters from independent normal distributions. The starting values from Table 3 were used as the means of the distributions and the standard deviations are derived from the suggested ranges (Table 3). The standard deviations of the proposal distributions vary dynamically during the chain progress through a tuning parameter (scale). This scale parameter is allowed to increase when the proposed move is rejected and is reduced when a move is accepted. This usually results in a reasonable acceptance rate. We chose not to include strong priors on the estimation method, but this could be incorporated in a future version. The chains were run for 10,000 iterations (Fig. S2). For calculating summary statistics we used a burn-in period of 1000 iterations. The convergence of the algorithm was assessed visually and also using Gelman diagnostics (Gelman et al., 2004) with a value between 1 and 1.2 considered as acceptable. In addition, the model efficiency (see statistics) was also used to evaluate the agreement between simulations and observations. The R code is available upon request.

2.3.5. Calibration protocols

We performed three types of calibration in order to judge the performance of the code, get a better understanding of how parameters interact among each other and provide suggestions for appropriate use of the code:

1. manual or hand-calibration in which the following parameters were allowed to change, if needed: a_3, $[a_4 + a_5]$, P_{crit1}, P_{sen1}, P_{crit2}, and P_{sen2} within a reasonable range (±15% for P_{crit} and P_{sen}, ± 5 d for a_3, and ±10 d for the combined $[a_4 + a_5]$ parameter). The manual calibration was done first and used later to judge whether the MCMC procedure provided reasonable estimates.
2. automated calibration in which two parameters were set for optimization: a_3 and $[a_4 + a_5]$. When the model fit was satisfactory (judged by the Gelman diagnostics and other statistical criteria described below) then the optimization process was ended.
3. automated calibration in which three parameters were set for optimization: a_3, $[a_4 + a_5]$, and P_{crit}.

This protocol was followed for datasets 1, 2, 3, 4, 5, and 6 in which both flowering and maturity data were available (Table 2). For the datasets 7, 8, 9, and 10 in which flowering date was available (Table 2), we optimized the a_3 parameter only.

2.3.6. APSIM soybean model configuration

In total 280 simulations were conducted in APSIM soybean (version 7.4). Each simulation refers to a particular combination of sowing time, year, cultivar and location (Table 2). Because this study investigates phenology prediction under non-limiting conditions, the soil profiles used are not important. We developed APSIM soil profiles (necessary to run simulations) for each location similarly to Archontoulis et al. (2014). We applied irrigation when necessary (e.g. Missouri) to allow the crop to complete the cycle and we also relaxed the "node_sen_rate" parameter to avoid crop death due to total leaf senescence.

2.4. Statistics

The goodness of fit was assessed by calculating the root mean square error (RMSE, the lower the value the better), the relative absolute error (RAE, the lower the value the better) and the modelling efficiency (ME, the higher the value the better). The equations can be viewed in Archontoulis and Miguez (2013) and for more details see Wallach et al. (2006).

3. Results

3.1. The proposed methodology

Table 4 shows that our methodology to calibrate the APSIM soybean phenology module is robust and works well, irrespectively of the calibration method used (manual versus automated). Both calibration methods resulted in substantial improvements in soybean phenology prediction compared to the uncalibrated model (Table 4). On average across the entire dataset ($n = 280$), RAE was below 1%, and the RMSE was 3.3 d and 6.1 d for flowering and physiological maturity, respectively. The ME was 0.90 and 0.87 for flowering and physiological maturity, respectively.

3.2. Manual versus automated calibration

The automated calibration methods although being constrained by the number of parameters to optimize (see 2.3.5 section)

Table 3
Starting values used for manual and automated model calibration. MG = maturity group, P_{crit} = critical photoperiod, P_{sen} = photoperiodic sensitivity, a_j = optimum days (for details see Table 1). Initial parameter values were taken from Boote et al. (2003). The a_j parameters were re-analyzed (sensitivity analysis and preliminary calibration using the data set# 2 from Table 2) to fit APSIM phenological phases.

MG	P_{crit}	P_{sen}	a_1	a_2	a_3	a_4	a_5	a_6
	(hour)	(1/hour)	Optimum days (d)					
00	14.35	0.148	5	5	5.0	11.2	22.8	1
0	14.10	0.171	5	5	5.6	11.7	23.8	1
I	13.84	0.203	5	5	6.0	11.9	24.2	1
II	13.59	0.249	5	5	6.4	12.3	25.0	1
III	13.40	0.285	5	5	8.0	12.7	25.7	1
IV	13.09	0.294	5	5	9.5	13.2	26.7	1
V	12.83	0.303	5	5	11.5	13.5	27.5	1
VI	12.58	0.311	5	5	12.5	13.9	28.2	1

performed equally or better compared to the manual calibration as indicated by the summary statistical indexes (Table 4). Examination of the statistical indexes for each individual dataset did not reveal a consistent pattern (as a function of number of data or location) that would explain why the manual method performed better in some cases and the automated method performed better in others. Most likely the inclusion of additional parameters in the manual calibration provided the model with advanced flexibility in fitting the data. However, given the restrictions imposed by a manual calibration (i.e. difficult to replicate, time consuming, tedious, requires skilled knowledge, and the fact that a good fit was achieved by adjusting only two or three input parameters) we propose use of the automated methods. In this way good behaviour of the model is ensured.

Between the two automated methods, the 3-parameter estimation was slightly superior compared to the 2-parameter (Table 4), but it was not a substantial improvement. Chain convergence according to the Gelman diagnostics tended to be better in the 2-parameter vs. the 3-parameter method. It is very

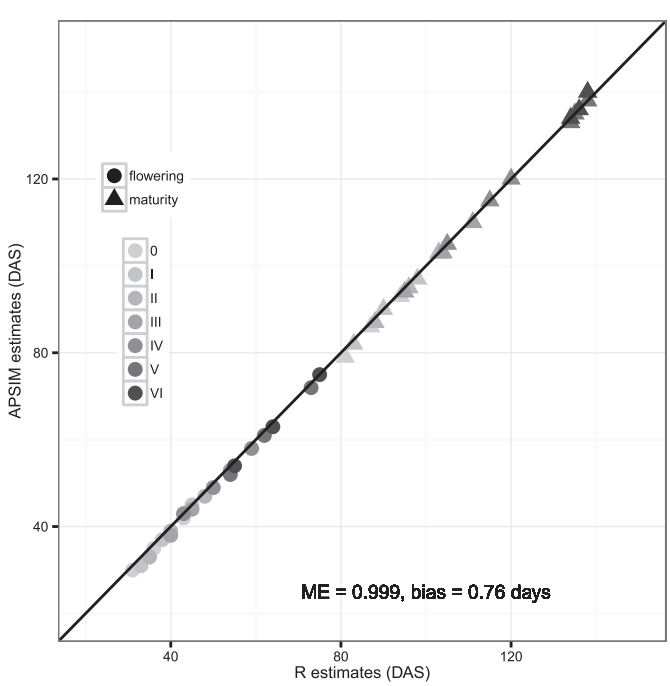

Fig. 2. Comparison of estimated days to flowering and to physiological maturity from the APSIM model and the R code for a particular dataset (Edwards and Purcell, 2005; $n = 2 \times 24 = 48$ data-points). Different symbols and colours refer to different phenological stages and maturity groups, respectively.

Table 4
Evaluation of goodness-of-fit among uncalibrated (using starting values from Table 3), manual calibrated and two automated calibration methods. In the manual calibration, the parameters a_3, $[a_4 + a_5]$, P_{crit1}, P_{crit2}, P_{sen1} and P_{sen2} were allowed to change within a reasonable range (see 2.3.5 section in the M&M). In the automated 1 calibration, the parameters a_3 and $[a_4 + a_5]$ were set for optimization. In the automated 2 calibration, the parameters a_3, $[a_4 + a_5]$ and P_{crit} were set for optimization. ME = modelling efficiency; RMSE = root mean square error; RAE = relative absolute error.

Set#	Calibration method	Flowering			Physiological maturity		
		ME (0–1)	RMSE (d)	RAE (%)	ME (0–1)	RMSE (d)	RAE (%)
1	Uncalibrated	−0.95	8.49	9.13	−2.80	15.77	9.55
	Manual	0.91	1.79	0.75	0.96	1.56	0.50
	Automated 1	0.86	2.23	0.79	0.90	2.53	0.48
	Automated 2	0.89	2.02	0.44	0.90	2.47	0.06
2	Uncalibrated	0.84	5.71	2.41	0.88	7.23	0.59
	Manual	0.86	5.43	2.10	0.93	5.48	0.25
	Automated 1	0.86	5.37	1.74	0.93	5.51	0.49
	Automated 2	0.89	4.76	1.40	0.97	3.90	0.38
3	Uncalibrated	0.24	11.84	21.4	0.65	10.44	6.69
	Manual	0.97	2.37	1.46	0.92	5.18	0.41
	Automated 1	0.97	2.52	0.73	0.88	6.23	3.04
	Automated 2	0.97	2.38	1.90	0.85	6.88	2.95
4	Uncalibrated	−3.70	14.62	28.78	−0.44	14.53	10.05
	Manual	0.34	5.45	4.43	0.87	4.39	0.68
	Automated 1	0.64	4.01	3.41	0.90	3.83	0.88
	Automated 2	0.68	3.79	3.60	0.92	3.38	0.90
5	Uncalibrated	−0.04	8.87	16.44	0.77	7.02	0.39
	Manual	0.87	3.11	0.81	0.74	7.52	0.37
	Automated 1	0.90	2.74	3.39	0.80	6.72	0.54
	Automated 2	0.91	2.66	2.24	0.84	6.02	0.02
6	Uncalibrated	−1.43	10.25	18.94	−3.01	20.61	16.77
	Manual	0.91	1.97	0.52	0.49	7.35	0.91
	Automated 1	0.91	2.06	0.76	0.57	6.73	0.38
	Automated 2	0.88	2.31	1.57	0.54	6.96	1.11
7	Uncalibrated	−0.01	8.16	16.14	–[a]	–	–
	Manual	0.78	3.79	1.82	–	–	–
	Automated 1	0.77	3.86	2.03	–	–	–
	Automated 2	nd[b]	nd	nd	–	–	–
8	Uncalibrated	−0.05	5.71	10.23	–	–	–
	Manual	0.95	1.29	0.62	–	–	–
	Automated 1	0.85	2.16	2.57	–	–	–
	Automated 2	nd	nd	nd	–	–	–
9	Uncalibrated	−2.61	5.70	4.28	–	–	–
	Manual	1.00	0.00	0.00	–	–	–
	Automated 1	0.94	0.71	1.21	–	–	–
	Automated 2	nd	nd	nd	–	–	–
10	Uncalibrated	0.27	7.80	15.07	–	–	–
	Manual	0.88	3.12	1.51	–	–	–
	Automated 1	0.90	2.93	3.86	–	–	–
	Automated 2	nd	nd	nd	–	–	–
All	Uncalibrated	0.13	10.08	17.32	0.63	10.25	3.82
	Manual	0.88	3.68	0.71	0.84	6.67	0.33
	Automated 1	0.91	3.25	2.17	0.87	6.01	0.35
	Automated 2	0.92	3.08	2.34	0.89	5.55	0.66

[a] No data available for physiological maturity (Table 2).
[b] The a_3 parameter was optimized (automated 1) when only flowering data were available.

likely that in order to optimize three parameters more with in-season phenological observations are needed for a more robust estimation. When flowering data were available, then we optimized only the a_3 parameter (Table 1). In general, if datasets with a narrow range of environments are used, the parameters that determine photoperiod response in soybean (P_{crit} and P_{sen}) are not likely to be robust enough for use in environments outside the calibration range.

In this study we provide estimates derived from the 3-parameter (sets 1, 2, 3, 4, 5 and 6) and 1-parameter (sets 7, 8, 9, 10) optimization method. Table 5 presents the parameter estimates for 40 soybean cultivars and Table S3 (in supplementary materials) the associated confidence intervals. Fig. 3 compares starting and

Table 5
Phenological parameter estimates (the confidence intervals are given in the Supplementary Table S3) for 40 soybean cultivars derived from the automated calibration methods. MG = maturity group, P_{crit} = critical photoperiod, P_{sen} = photoperiodic sensitivity, a_j = optimum days (for details see Table 1). Empty cells indicate lack of physiological maturity data.

MG	Cultivar name	Parameters					Set
		P_{crit}	P_{sen}	a_3	a_4	a_5	
		(hour)	(1/hour)	Optimum days (d)			
00	Trial[a]	14.430	0.148	3.40	10.80	21.62	2
0	Lambert[a]	14.293	0.171	4.68	11.04	22.11	2
0.8	Asgrow0801	14.243	0.197	2.15	11.95	23.93	4
1	IA 1006[a]	14.373	0.203	6.78	12.94	25.92	2
1	Pioneer 91B01	13.840	0.203	2.80	–	–	8
1.5	Dekalb1552	14.517	0.226	4.51	15.12	30.29	4
2	IA 2008[a]	13.917	0.249	6.47	14.49	29.02	2
2	K-283	13.590	0.249	2.97	–	–	7
2.5	U01390224	14.070	0.267	3.79	15.23	30.51	4
2.6	Pioneer 92M61	13.771	0.271	3.54	13.14	26.32	3
2.7	Krucr	13.864	0.274	6.54	12.58	25.54	1
2.7	Elgin	13.573	0.274	3.68	11.69	23.73	1
2.8	HiSoy 2846	13.438	0.278	10.1	–	–	9
3	Wayne	13.544	0.274	7.87	10.75	21.83	1
3	Macon[a]	14.050	0.285	8.35	15.16	30.36	2
3	NE3001	13.403	0.285	3.12	12.64	25.31	4
3.1	Average[b]	13.628	0.286	2.21	13.27	26.57	4
3.2	Becks 321NRR	13.451	0.287	3.62	12.96	25.96	3
3.2	Average[c]	13.606	0.287	1.98	13.31	26.66	4
3.3	Average[d]	13.464	0.288	1.53	13.24	26.52	4
3.4	Average[e]	13.463	0.289	4.57	12.11	24.25	4
3.4	Average[f]	13.553	0.289	3.81	15.67	31.39	5
3.4	Pioneer 93M42	13.276	0.289	4.53	–	–	9
3.5	Average[g]	13.299	0.290	4.08	11.97	23.98	6
3.6	Stine	13.650	0.290	8.09	12.13	24.62	1
3.6	U98307162	13.298	0.290	4.81	12.54	25.13	4
3.7	Becks 367NRR	13.265	0.291	3.33	12.63	25.31	3
3.9	Williams	13.438	0.293	6.70	12.05	24.46	1
3.9	U98311442	13.355	0.293	4.00	12.29	24.61	4
3.9	Average[f]	13.339	0.293	5.30	15.68	31.41	5
4	Pioneer 94B01[a]	13.054	0.294	6.12	14.16	28.35	2
4	Average[h]	13.090	0.294	4.62	–	–	10
4.2	Dekalb4251	13.482	0.296	3.79	15.90	31.84	4
4.4	Average[f]	13.206	0.298	6.57	15.94	31.92	5
4.9	Average[f]	13.118	0.302	8.25	16.45	32.95	5
5	Hutcheson[a]	12.575	0.303	11.9	12.61	25.25	2
5	Average[i]	12.830	0.303	10.2	–	–	10
5.4	Average[f]	12.899	0.306	8.67	16.55	33.15	5
5.9	Average[f]	12.724	0.310	10.3	16.10	32.24	5
6	NK 622[a]	12.392	0.311	11.8	11.67	23.37	2

[a] The listed cultivars were used in all the experimental years: 2001, 2002 and 2003. In 2002, the researchers used two cultivars for each maturity group. The additional cultivars used in 2002 were: Jim (MG OO), AC Comoran (MG O), MN 1801 (MG 1), Dwight (MG 2), Pana (MG 3), MPV 437 (MG 4), Caviness (MG 5) and Desha (MG 6). For details, see Edwards and Purcell (2005).
[b] Average parameter values from three cultivars: Dekalb 3152, Latham 1067RR and NEX8903.
[c] Average parameter values from two cultivars: Krueger 323RR and NE3201.
[d] Average parameter values from two cultivars: KAUP 335 and Pioneer 93B63.
[e] Average parameter values from three cultivars: Asgrow 3401, Pioneer 93B47 and Stine 3632.
[f] Average parameter values from many cultivars (see Table 2 in Zhang et al., 2004).
[g] Average parameter values from 14 cultivars: Asgrow AG3401 (MG 3.4), Dekalb DKB 31-52 (MG 3.1), Kaup 335 (MG 3.3), Kruger K323 + RR (MG 3.2), Latham 1067RR (MG 3.1), NE3001 (MG 3.0), NE3201 (MG 3.1), NEX8903 (Mg 3.1), U98-307162 (MG 3.4), U98-307917 (MG 3.4), U98-311442 (MG 3.9); Pioneer 93B36 (MG 3.3), Pioneer 93B47 (MG 3.4), Stine 3632-4 (MG 3.6).
[h] Average parameter values from two cultivars: Asgrow AG4403 and Hombeck HBK4891.
[i] Average parameter values from two cultivars: Asgrow AG5701 and Pioneer P9594.

final parameter estimates. The final parameters tended to have higher P_{crit} values (about 0.22 h), lower a_3 values (about 2.5 d), higher $[a_4 + a_5]$ values (about 1.4 d) compared to the starting values.

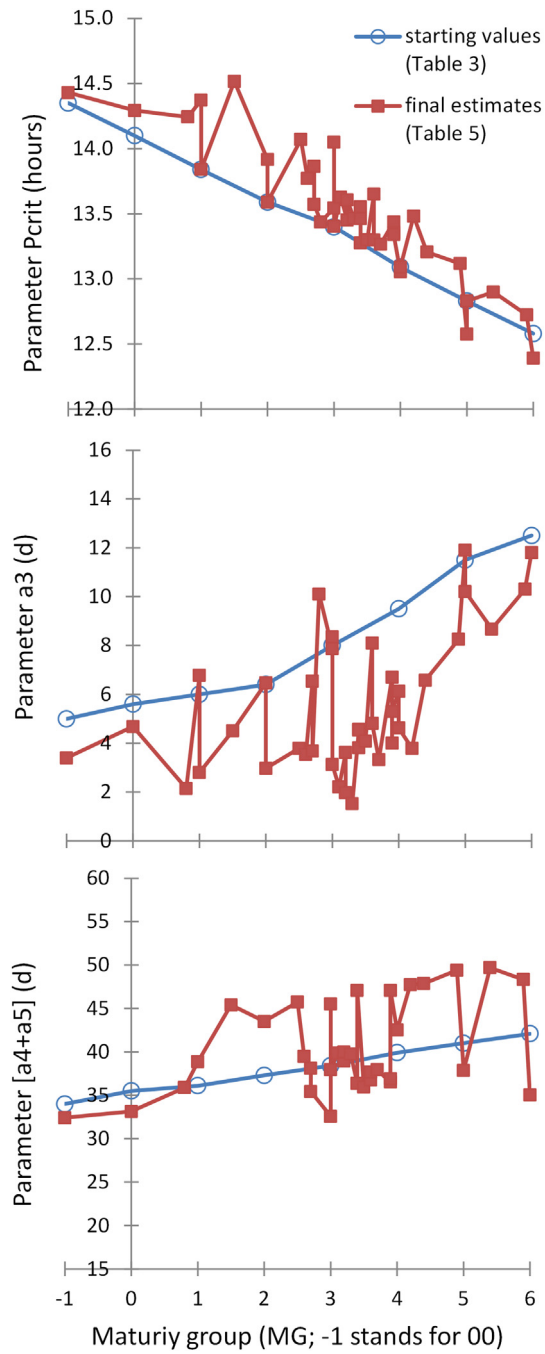

Fig. 3. Comparison between starting values and final estimates for three parameters: P_{crit} (critical photoperiod; top panel), a_3 (optimum days from floral initiation to flowering; middle panel), and $[a_4 + a_5]$ (optimum days to complete the grain fill period; lower panel).

3.3. Flowering

Fig. 4 illustrates the goodness of fit for the flowering data across a range of environmental conditions (Table 2). The distribution of the data around the 1:1 line did not indicate any bias. In general, the model simulated flowering DAS with an RMSE of 3 d and RAE of 2.3%. Among the datasets, some difficulties were encountered in fitting the data reported in set 5 (Zhang et al., 2004); which is attributed to the fact that these data represent average values across four experimental years for a number of cultivars.

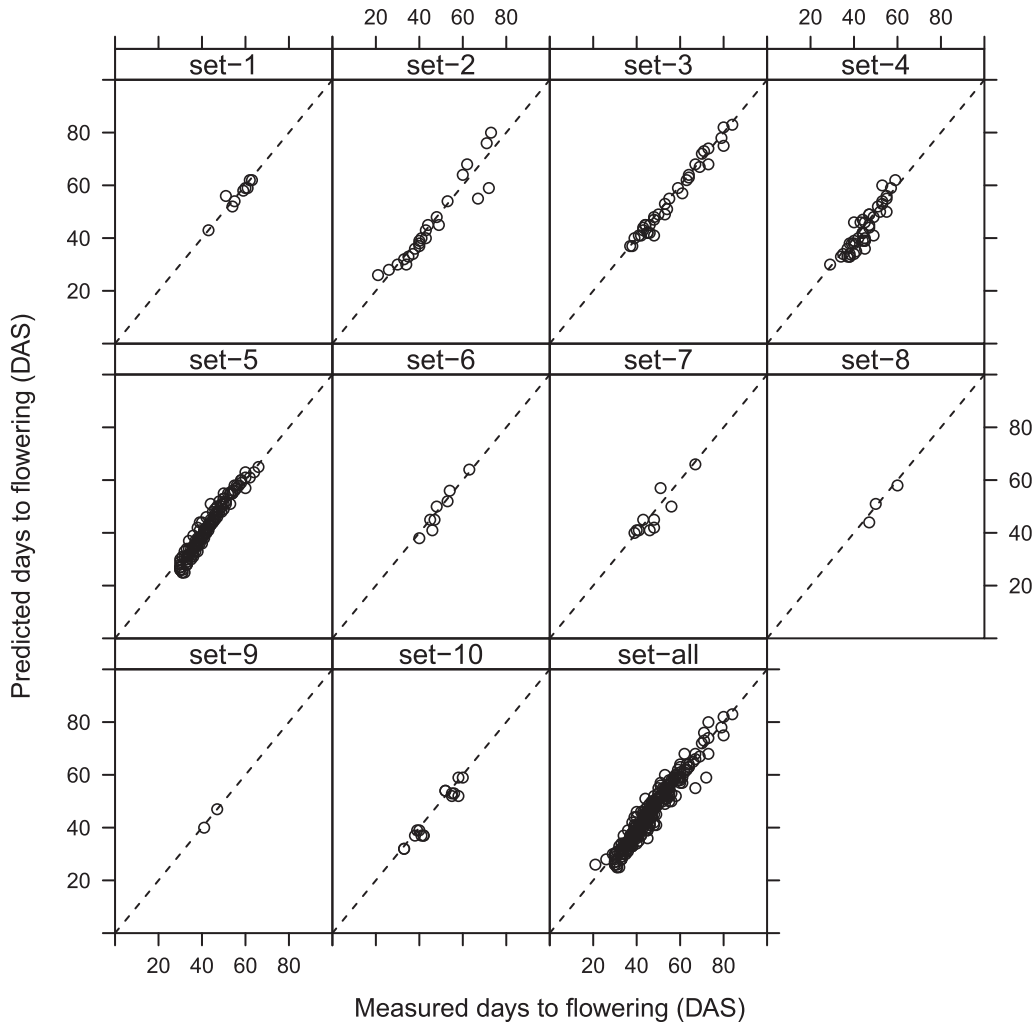

Fig. 4. Simulated versus measured days to flowering (as days after sowing; DAS) for each experimental dataset (see Table 2 for references) including also a summary plot. The diagonal dotted lines are 1:1. Statistics are presented in Table 4.

3.4. Physiological maturity

Fig. 5 illustrates the agreement between simulated and observed DAS to physiological maturity. The model performed very well in all cases (RAE = 0.6%), except Indiana (Robinson et al., 2009) and Mississippi (Zhang et al., 2004), in which a systematic underestimation and a large variability around the 1:1 line were detected, respectively. In these two datasets the RMSE was 6.8 d and 6.0 d, respectively, still close to the average RMSE of 5.5 d. For the Indiana dataset the manual hand-calibration method resulted in better fits (Table 4) indicating that use of different P_{crit} and P_{sen} parameters for pre- and post-flowering phases in some cases might be important.

3.5. Start grain filling

Our optimization code utilizes the assumption that the physiological days (a_4 parameter) to complete the FL_SD phase are about 33% of the physiological days ($a_4 + a_5$ parameter) to complete the combined FL_SD + SD_END phase. We preferred relying on this assumption and optimizing the combined [$a_4 + a_5$] parameter rather than keeping one parameter constant and optimizing the other one when no information exists for the start grain fill phase. Fig. 6 illustrates grain dry matter accumulation over time (observed versus simulated data from set 1) and shows that our assumption is reasonable for maturity groups from 2.7 to 3.9. A common problem in evaluating this stage precisely is that field observations on seed weight are usually taken every 2–3 weeks, which makes the estimation of this particular day quite difficult (Fig. 6). In general, accurate quantification and prediction of the start grain fill stage has more uncertainty associated with it compared to the uncertainty in flowering or physiological maturity stages (see Section 4.3).

3.6. Predicted soybean adaptability and productivity in the USA

Fig. 7 illustrates simulated flowering, physiological maturity and relative yield for eight soybean maturity groups across three locations. The model predictions are in accordance with what is known for soybean adaptability and productivity in different locations across USA (e.g. Zhang et al., 2007; Pedersen, 2009). In this sensibility test we used default parameter values for different maturity groups, which can be regarded as "generic coefficients" (Table 3). When we repeated the simulation exercise by considering slightly different starting values based on the trends indicated in Fig. 3 (see also Section 3.2), the simulated patterns did not vary much. For the relative seed yield predictions, we had set the cultivar specific parameters "y_hi_incr" and "y_hi_max_pot" to 0.01 (d^{-1}) and 0.5 ($g\ g^{-1}$), respectively across cultivars. In other words, only the phenological parameters were varied among the soybean cultivars.

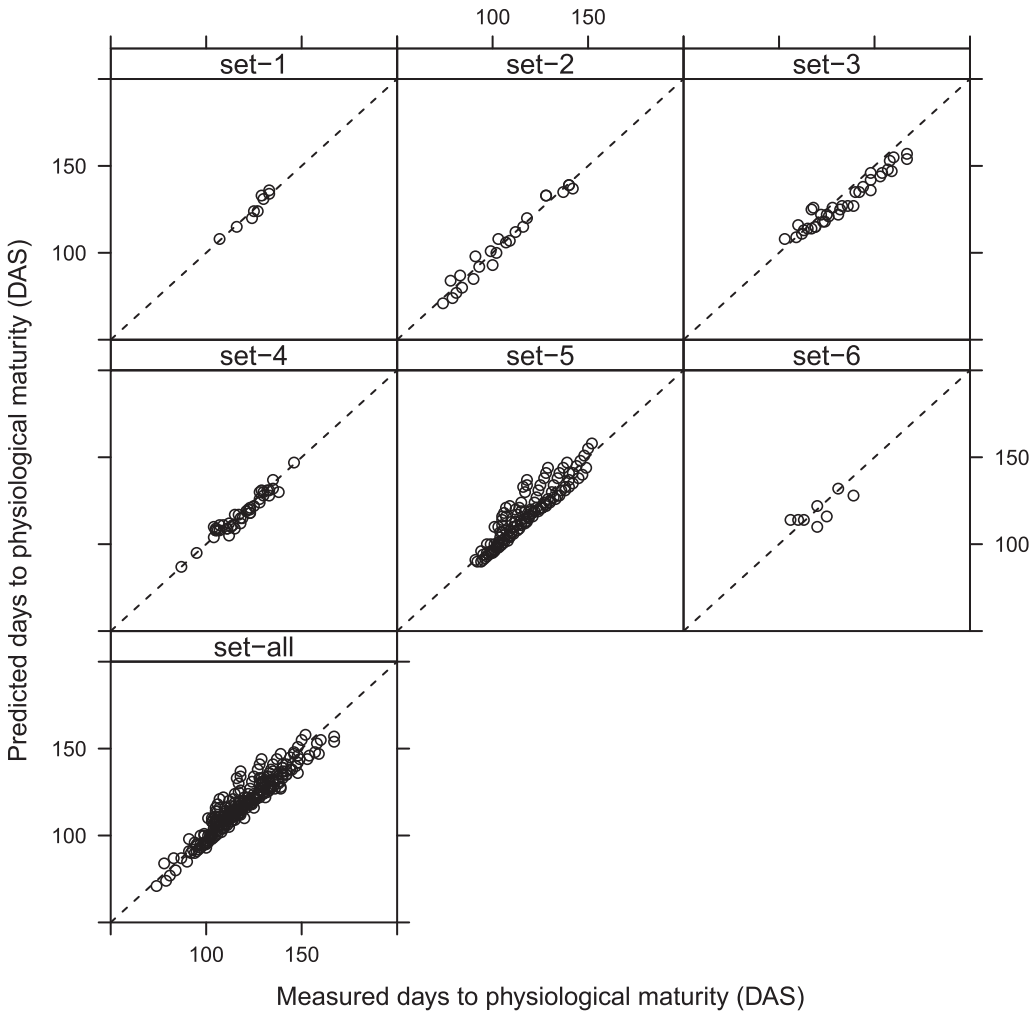

Fig. 5. Simulated versus measured days to physiological maturity (as days after sowing; DAS) for each experimental dataset (see Table 2 for references), including also a summary plot. The diagonal dotted lines are 1:1. Statistics are presented in Table 4.

4. Discussion

4.1. Towards simplifying phenology calibration

In line with the general effort towards simplifying calibration of phenological modules (Mavromatis et al., 2001; Setiyono et al., 2007; Jones et al., 2011), we developed a new methodology and an MCMC approach that can be used to derive parameter estimates to facilitate parameterization of the multiple input parameter phenology module (generic PLANT) within the APSIM simulation platform. We showed that prediction of soybean development stages (Figs. 4–6) can be achieved by using information on maturity group, flowering and physiological maturity only, information which should be readily available. The proposed methodology is expected to assist calibration of all the short-day species included in the APSIM PLANT platform, and especially legumes. Some parameters developed for soybean have the potential to be shared with other legume species following the approach of Wang et al. (2002). In general, this study expands the application potential of the APSIM-soybean model.

Our parameter estimates for 40 soybean cultivars differ from the initial starting values (Fig. 3). The departures from the initial starting values were not consistent and largely cultivar specific, e.g. see the data scatter for the cultivars belong to the maturity group 3 (Fig. 3). In future soybean phenology calibration exercises we recommend users to start over with the values reported in Table 3 (generic coefficients) and estimate cultivar specific parameters using the automated methods. When the manual calibration is used, the trends showed in Fig. 3 can help users to identify cultivar specific parameter values. In case of no prior available information, users can use the starting values (Table 3) for a good approximation of the soybean phenological stages across regions and maturity groups (Fig. 7).

4.2. Evaluating phenology predictions

In evaluating the performance of the model, it is necessary to consider uncertainties associated with the observed data. In this study, we can identify uncertainty associated with the spatial error due to field variability and temporal error due to the discontinuity of the Fehr and Caviness (1977) soybean staging system which was used to assign phenological events in the field. In addition, there is one more source in our study, which is the uncertainty associated with the interpretation of the published data, especially for the data extracted from figures (e.g. Robinson et al., 2009), and the fact that some published data were reported as average values across MG or years (e.g. Zhang et al., 2004).

Given these uncertainties, the overall performance of the model is characterized as very good (Table 4). The observed RMSE values (about 3 d for flowering and 6 d for maturity predictions) were close to RMSE values reported in soybean phenology prediction

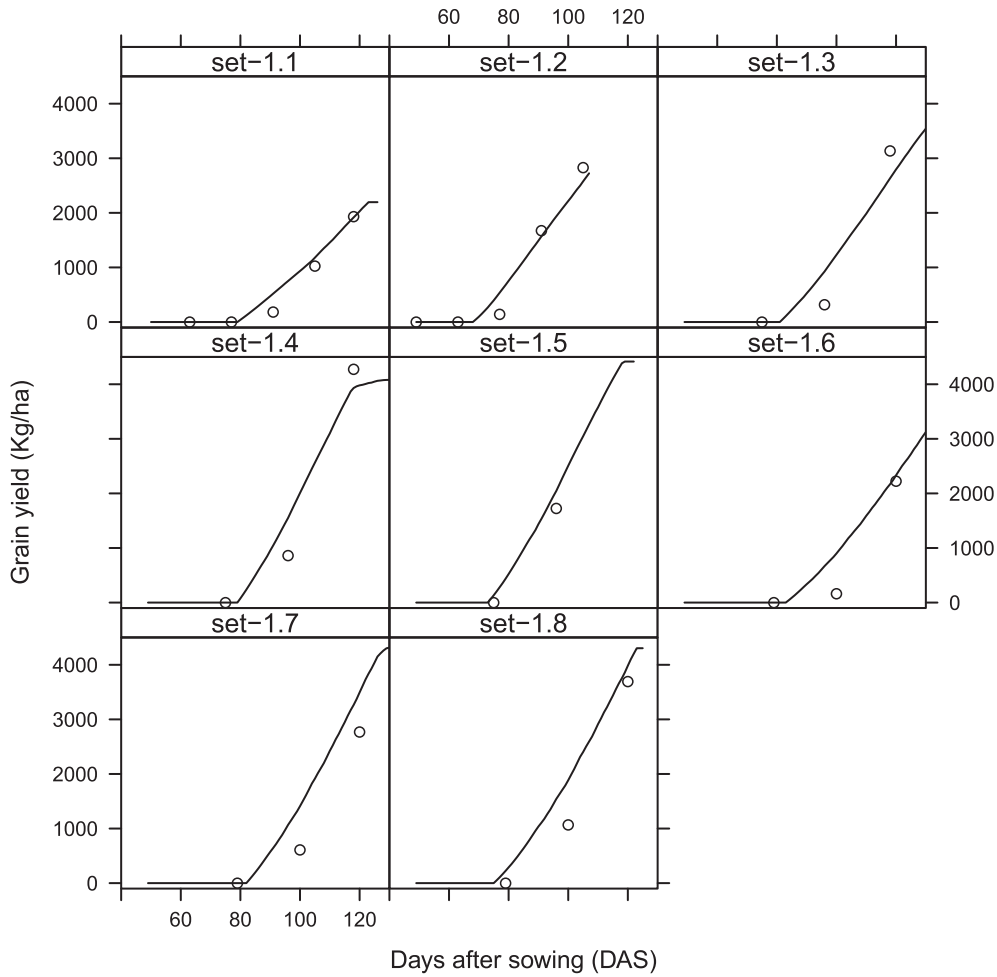

Fig. 6. Measured (cycles) and APSIM simulated grain yield (lines) over time for eight experiments conducted in Iowa covering a range of soybean maturity groups from 2.7 to 3.9. Each panel refers to a combination of sowing time, cultivar, location and year (set 1 in Table 1; data from Hoogenboom et al., 2012).

studies (Mavromatis et al., 2001; Setiyono et al., 2007; Torrion et al., 2011; Jones et al., 2011). An advantage of our study over the aforementioned ones, is the wide range of environments used for calibration (from 33° to 46°N; $n = 280$; Table 2).

In this study, we did not follow the traditional scheme of dividing the data into calibration and validation sets. Instead, we used the entire database to develop robust phenological parameters and to demonstrate the functionality of the proposed methodology. We evaluated only goodness of fit. Similar approaches have been used in the literature (Carberry et al., 2001; Turpin et al., 2003; Farre et al., 2004).

4.3. Assumptions and recommendations

In the literature, data on flowering and physiological maturity are largely available; data on the start of seed filling are sporadically available while data on the end of juvenile and floral initiation are very rare. For this reason our methodology and optimizer were built around flowering and maturity data. It should be noted that the optimization code allows incorporation of additional phenological observations if they exist.

One difficulty noted in this study was the correct interpretation of the start of seed filling stage. According to the most commonly used staging system for soybean (Fehr and Caviness, 1977), the R4 stage (pod is 2 cm long) marks the beginning of the start of seed fill period and the R5 stage (seed is 3 mm long) indicates the beginning of the linear phase in seed filling (rapid accumulation of dry matter; see Fig. 6). Recording the dates of R4 or R5 requires the observer to make a quantitative assessment of pod length or seed diameter, whereas the potential intrinsic error might be significant in the field (Torrion et al., 2011). In general, for the majority of crop species, use of morphological observations (e.g. seed diameter) to approximate seed physiological activity (seed weight) is associated with large uncertainty (e.g. Archontoulis et al., 2010). Introducing such uncertainty into crop models is risky. Therefore, we did not include morphological data on the start of grain fill period in our analysis, which data were available in some studies (Zhang et al., 2004; Bastidas et al., 2008; Robinson et al., 2009, Table 2). Instead, we merged the FL_SD and SD_END phase into one phase and estimated the combined $[a_4 + a_5]$ parameter (Table 1). The value of 0.33 was later used to partition the combined parameter into a_4 and a_5. This value was derived from a sensitivity analysis and proved to be reasonable for soybean MG from 2.7 to 3.9 (Fig. 6) as well as for all the MG according to a sensibility test (Fig. 7). The choice of this partitioning parameter is critical for accurate estimation of seed yield.

APSIM makes a distinction between the end of seed fill period and physiological maturity (Eq. (1)), while many other models assume that these two phases coincide (SOYDEV; CROPGRO-soybean). Data to directly evaluate this stage were not available, so an arbitrary value of one physiological day was assumed for the parameter a_6 (Table 1). This parameter has little impact on phenology prediction and should be considered as an option during

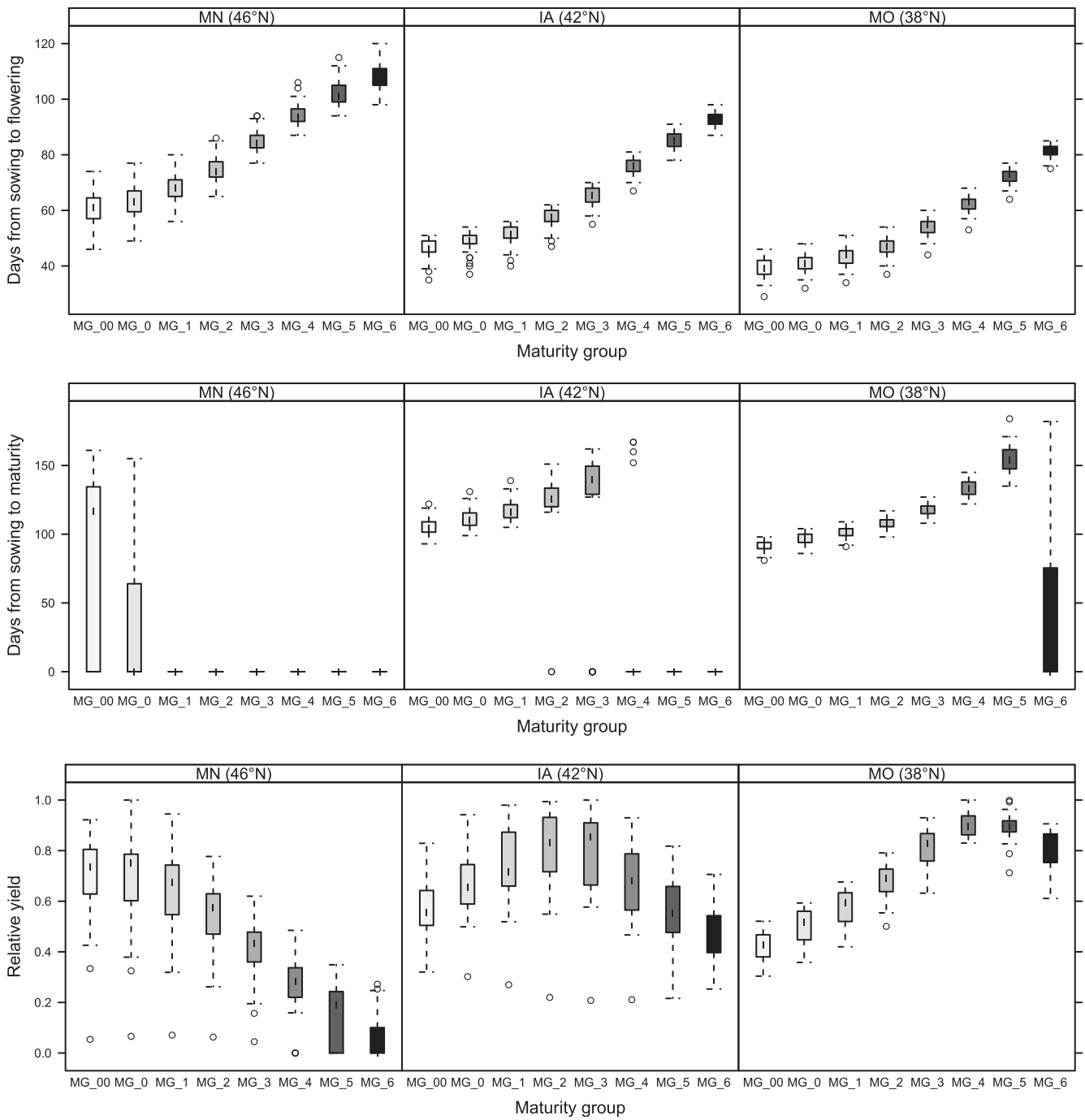

Fig. 7. Predicted soybean adaptability (upper panel: flowering time; middle panel: physiological maturity) and productivity (lower panel: relative yield; with 1 being the maximum yield) for eight maturity groups (MG) in three USA States (MO: Missouri; IA: Iowa; MN: Minnesota) using the updated APSIM-soybean model. Sowing time was May 10 in all locations and irrigation applied in Missouri only. The length of each box indicates the variability in model predictions created by replicating the simulation exercise for 32 years (1980–2011). Invisible bars or bars touching the *x*-axis in the middle panel, indicate that the physiological maturity was not reached or high risk of failure, respectively.

the second stage of model calibration which is fitting the yielding data. If the simulated yield is higher than the observed, an option is to increase the a_6 and at the same time to decrease the $[a_4 + a_5]$ by approximately the same amount to maintain a good prediction of physiological maturity.

4.4. The potential of the optimization algorithm

The way that the R code was written allows researchers to explore a number of hypotheses related to temperature × photoperiod interactions in short day species and especially soybean. Depending on the research objective and data available, they can optimize with minor modifications in the R code any of the following parameters: T_b, T_o, T_m, sun_angle, P_{crit}, P_{crit1}, P_{crit2}, P_{sen}, P_{sen1}, P_{sen2}, a_1, a_2, a_3, a_4, a_5 and a_6 (Table 1), as well as the shape of the temperature response function (Fig. S1 in the supplementary materials). It can facilitate phenology prediction up to flowering or throughout the cropping cycle. The R code can be modified to estimate parameters for long day species, can be extended to account for vernalization and/or water stress effects on phenology.

The optimization tool was built outside the APSIM platform (stand-alone tool in R), meaning that it can be also used by

individual researchers to examine scientific hypotheses or to estimate phenological parameters for short-day species of interest independently of a simulation model.

Our optimization code was designed to read similar input files as those used by DEVEL2 (Holzworth and Hammer, 1996) to allow data exchange between the two optimizers. The differences between the proposed optimizer and DEVEL2 are: a) captures the whole crop life cycle and accounts for temperature × photoperiod interactions throughout the crop cycle (Eq. (1)), while DEVEL2 had been applied to predict phenology up to flowering stage (Kumar et al., 2009; Cave et al., 2013 for recent applications); b) utilizes the thermal time approach and includes 3 options for temperature response functions, while DEVEL2 includes both thermal time method and the multiplicative method and 9 options for temperature response functions; c) utilizes stochastic methods in parameter estimation (Markov chain Monte Carlo algorithm), while DEVEL2 uses the simplex method; and d) our code is written in R while DEVEL2 is in FORTRAN 77.

4.5. Limitation of the current approach

The present methodology and the optimizer do not include (water and nitrogen) stress effects on the rate of development although such an effect may exists (Brevedan and Egli, 2003; Setiyono et al., 2007 and references therein). Theoretically, it requires observations to be made under non-limiting conditions in order to obtain robust parameter values. If stress has occurred during plant growth and has affected the rate of development, then the estimation process will attempt to set parameter values to compensate for water, nutrient, pest or disease stresses (Jones et al., 2011). The majority of the observed data used in this study (Table 2) were collected under field conditions in which pest or diseases had been controlled efficiently. Field experiments were well irrigated in southern US States and Nebraska or conducted in areas with sufficient precipitation for soybean growth (US Midwest). Therefore, it is believed that our parameter estimates for soybean are robust (Table 5).

5. Conclusions

We demonstrated a potential avenue towards calibrating a multi-parameter input phenological model that accounts for temperature × photoperiod interactions throughout the crop cycle, from readily available information on flowering and physiological maturity. By making use of an optimization tool and literature information we developed phenological parameters for 40 soybean cultivars covering maturity groups from 00 to 6 for the APSIM soybean model. Given that phenology captures much of the genotypic variation, the potential applicability of the APSIM-soybean model has been expanded significantly, which is of particular interest in the new era of crop model application; i.e. upscale process-based point models across regions. Our methodology and optimization code are generic, hence they can be applied to calibrate phenology of all the short-day species included in the APSIM PLANT model. Their combined use can also serve as a template towards developing calibration protocols in other modelling platforms.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.envsoft.2014.04.009.

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