

Determination of genetic coefficients of three spring wheat varieties under a Mediterranean environment applying the DSSAT model

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The impact of climate change requires developing and validating models that help to project possible scenarios that must adapt to new varieties. This study seeks to validate and calibrate the Decision Support System for Agrotechnology Transfer (DSSAT) model as a tool that facilitates the characterization of the behavior of new varieties in the face of new scenarios generated by climate change. The determination of genetic coefficients of three bread wheat (*Triticum aestivum* L.) varieties was considered in the methodology; this was done with the database of the historical records of the Instituto de Investigaciones Agropecuarias (INIA) Wheat Breeding Program for the 2000 to 2011 period. Once the adjustment level of the model was dealt with, it was feasible to obtain genetic coefficients of three spring wheat varieties (Pandora-INIA, Kipa-INIA, and Millán-INIA); days from planting to anthesis variable exhibited RMSE values fluctuating between 3.5 and 9.7 depending on the variety. For total duration of days to maturity, 'Millán-INIA' exhibited a very good adjustment (RMSE = 0.25) as compared to 'Pandora-INIA' (RMSE = 1.35) and 'Kipa-INIA' (12.22). Furthermore, the coefficient of determination of the genetic coefficients indicates that the varieties have minimum vernalization requirements; these are similar to the photoperiod between 'Pandora-INIA' and 'Millán-INIA' and lower in the case of 'Kipa-INIA'. Thermal requirements for grain filling, biomass production, and plant height did not exhibit any important differences among varieties. Finally, the methodology allowed calibrating the DSSAT model and achieving a good predictive level of yields for the three varieties. The plant development parameters must be studied in greater detail because of the low association between simulated and observed values.

Key words: Climate change, DSSAT model, genetic coefficients, simulation, *Triticum aestivum*.

INTRODUCTION

World agriculture is faced with the challenge of adapting to the consequences of climate change, a phenomenon affecting crop productive stability by reducing water availability for growth. In addition, the world population is constantly increasing and will reach 9600 million by 2050 according to United Nations projections (ONU, 2014). This will oblige the agricultural sector to increase its productive level to satisfy the growing demand for food, which is a complex problem to solve because of the multiple factors involved in agricultural production. It is therefore necessary to integrate technological tools that guide farmer decision making, for example, defining rotation or determining irrigation needs. Among these

available tools are simulation models that summarize the interaction between the different factors of the productive process and allow defining new scenarios to introduce changes in their variables. The usefulness of the models has generated a series of programs able to simulate crop development and production by using genotypic, environmental, and management information. One of these support tools is decision support system for agrotechnology transfer (DSSAT) that has been developed and used for the last 15 yr by researchers associated with agriculture in approximately 100 countries around the world (Jones et al., 2003). The DSSAT model consists of a set of independent programs that operate simultaneously on simulation models using information from the soil, climate, crop, and agronomic management databases (Uehara and Tsuji, 1998; Jones et al., 2003).

In order to function correctly, DSSAT needs a database related to the climate and soil of the study area, crop management, and information about the genotypes with respect to seven genetic coefficients that simulate the phenotypic expression of the genes under different environments (Boote et al., 2001), which can vary based on the duration of each growth stage within the crop's life cycle (Boote et al., 2001), and relating crop physiology

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Received: 29 December 2014.

Accepted: 7 May 2015.

doi:10.4067/S0718-58392015000500006

to environmental factors and agronomic management (Warnock et al., 2005). It is thus possible to characterize and determine the genetic differences between cultivars as well as the duration of the growth cycle and harvest index.

The DSSAT model needs to be calibrated and validated for each variety and region where it has previously been used. Warnock et al. (2005) point out that three steps are necessary to apply a model: calibration, validation, and application. Calibration provides the genetic coefficients with the best adjustment between simulated and observed data and is then validated by comparing it to a dataset of observed data different from those used in the calibration.

As in the rest of the world, Chile has been defined as a country that is vulnerable to the climate change phenomenon; according to the National Environmental Commission (CONAMA, 2008), agricultural activity would be one of the most affected. There also exists the need to increase efficiency by integrating and applying technologies that are able to support breeders in generating new varieties with respect to the climate conditions that the genotypes they develop must face and simultaneously guide farmer decision making in accordance with the available climatic and productive resources. Bread wheat (*Triticum aestivum* L.) in Chile is a very important cereal according to data from ODEPA (2014); this crop covered a total area of 238 410 ha during the 2012-2013 season and reached a national mean yield of 5.73 Mg ha⁻¹. The great variability of agroclimatic conditions in the production areas obliges conducting assays to evaluate the adaptation of the crop in each one of them. Therefore, according to studies carried out during the last 15 yr (Jones et al., 2003), validating the DSSAT model will allow the development of preliminary analyses of crop behavior for the different agroecological areas of interest and which include the conditions that would be generated as a result of the scenarios proposed by the IPCC (2013).

The objective of the present study was therefore to calibrate and validate the DSSAT model for three spring bread wheat varieties under Mediterranean climate conditions using historical climate, soil, and agronomic management databases of the area under study.

MATERIALS AND METHODS

The selected study site was INIA's Santa Rosa Experimental Station (36°36' S, 72°21' W) located in south central Chile; it has a Mediterranean climate (del Pozo y del Canto, 1999) with 1000 mm average annual precipitation and loamy soil texture with a 0.6 m depth of the Arrayán series corresponding to a Humic Haploxerands (USDA; Stolpe, 2006). Assay management was optimum with adequate fertilization, irrigation, and weed control for each season, and stress conditions were avoided.

The selected spring wheat varieties were 'Pandora-INIA', 'Kipa-INIA', and 'Millán-INIA', which are widely used in Chile; they were liberated between 2003 and 2012 with potential yields of 12 Mg ha⁻¹.

DSSAT model information requirements

This software was originally developed by an international network of scientists, cooperating in the International Benchmark Sites Network for Agrotechnology Transfer Project, motivated by a need to integrate knowledge about soil, climate, crops and management, for making better decisions about transferring production technology from one location to others where soils and climate differed (Uehara and Tsuji, 1998). The systems approach provided a framework in which research is conducted to understand how the system and its components function. This understanding is then integrated into models that allow one to predict the behavior of the system for given conditions (Jones et al., 2003).

The DSSAT model requires the creation of three databases; one corresponds to the physiological traits and agronomic management of each variety, as well as soil and climate information of the area selected for this study.

Crop characteristics database: Information used was of data observed in the assays developed by INIA's Wheat Breeding Program between the 2000 and 2012 seasons. Crop management information considered the following: planting date, emergence, flowering, physiological maturity and harvest, number of grains per spike, grain weight (mg), plants m⁻², number of stems m⁻², irrigation, planting depth, fertilization in each season, and crop yield (kg ha⁻¹).

To calibrate and validate the model, it is necessary to determine the genetic coefficients of each wheat genotype used in the study; therefore, all the genotypes were entered into the .CUL file extension. Seven genetic coefficients were considered of which three were related to crop development (P1V, P1D, and P5), three to growth (G1, G2, and G3), and one called phyllochron (PHINT) that involves the thermal time requirement for leaf appearance. These coefficients establish the genetic differences among cultivars and give an idea about the duration of the growth cycle and harvest index of each one. Rodríguez et al. (2010) describe each genetic coefficient as: days with optimum temperature for vernalization (P1V), percentage reduction in development rate with a photoperiod 10 h lower than the threshold (P1D), thermal time of grain filling stage (°C d) (P5), number of seeds per unit canopy weight at anthesis (#/g) (G1), normal seed size under optimum conditions (mg) (G2), normal dry weight (total, including grain) of one unstressed stem at maturity (g) (G3), and thermal time between appearance of successive leaves (°C d) (PHINT).

Soil and climate databases: Reports from the Natural Resources Research Center (Centro de Información de Recursos Naturales CIREN, Santiago, Chile) were used to construct the soil database and were included in the

DSSAT soil.sol file. Climate information was provided by the Automatic Meteorological Station of the Universidad de Concepción (36°35'43" S, 72°4'48" W) and corresponds to maximum and minimum temperatures, precipitation, and solar radiation. These data were entered in the WeatherMan module of DSSAT to generate WTH type files.

Description of varieties used

'Pandora-INIA', 'Kipa-INIA', and 'Millán-INIA' are spring wheat (*Triticum aestivum* L.) cultivars created by the Wheat Project at Instituto de Investigaciones Agropecuarias, INIA Quilamapu, Chillán, Chile. 'Pandora-INIA' was starting from a cross made in 1989. It is a semi-dwarf wheat with a plant height of 90-95 cm. The grain is brown and ovate. The spike is white and bearded. In trials its grain yield has varied between 7.5 and 10.8 t ha⁻¹. The average bread volume, sedimentation value, and grain protein were 722 cm³, 41.6 cm³, and 11.1% respectively, which classified this cultivar for direct use in bread making. 'Kipa-INIA' has an upright growth habit in the seedling stage. The adult plant is low to medium height and varies between 90 and 95 cm. The spike is white with long awns along its full length. The grain is ovate, white, and vitreous. It was sown in mid-August in the Santa Rosa Experimental Field (36°31' S; 71°54' W), Chillán, head emergence occurred 90 to 95 d after sowing, i.e. 4 to 6 d before 'Domo-INIA'. On the mean, 'Kipa-INIA' sown under irrigation conditions reached a yield of 11.7% higher than the control 'Domo-INIA', and 18.1% higher in dryland soils. 'Millán-INIA' is a variety originated from a cross carried out in 1995. This is a variety with an early to medium-early head emergence and upright growth habit in the seedling stage. The adult plant is low to medium height and varies between 75 and 90 cm, with a mean of 85 cm. The spike is white with long awns along its full length. The grain is large-sized, white, and vitreous. The weight of 1000 grains varies between 50 and 59 g. It was sown in mid-August at the Santa Rosa Experimental Station. Head emergence occurred 88 to 89 d after sowing. On average, 'Millán-INIA' reached a yield similar to that of 'Ciko-INIA'. This line stands out for its good resistance to disease, high protein content (11.5% mean), high sedimentation value, and high W value.

Implementation of DSSAT, use of GLUE, model calibration, and evaluation

The DSSAT model v.4.5 was used to perform this analysis. Three files were created for each variety, that is, .WHX, .WHT, and .WHA. Crop information from the ATCreate module was included to create three files; the first is .WHX, an experimental file containing detailed information of the experimental conditions such as environmental characteristics, soil analysis, initial soil moisture and N conditions, seedbed preparation and planting distance, irrigation and water management,

fertilization, agrochemical applications, and harvest. On the other hand, the .WHT file integrates the evolution of the field data over time, and the .WHA file contains yield information, anthesis date, and number of spikes m⁻² (Hoogenboom et al., 2003).

The genetic coefficients were then calculated for each cultivar with the DSSAT GLUE (Generalized likelihood uncertainty estimation) method. It should be noted that GLUE is a Bayesian estimation method to determine the probability distribution between observed data and those estimated by the model (He et al., 2010). Coefficients whose values exhibit the best adjustment were copied to the DSSAT CUL file to apply them in the program routines and evaluate the model (He et al., 2010).

Calibration of DSSAT model

The model was calibrated with field information from different seasons for each variety. Thus, information from the 2003, 2005, 2008, 2009, and 2010 seasons was used for 'Pandora-INIA', 2006, 2008, and 2010 seasons for 'Kipa-INIA', and 2005, 2006, and 2011 seasons for 'Millán-INIA'. Subsequent validation was performed for the three wheat varieties with different years. The years considered were 2000, 2001, 2002, 2004, 2006, and 2007 for 'Pandora-INIA', 2005, 2007, 2009, and 2011 for 'Kipa-INIA', and 2007, 2009, and 2010 for 'Millán-INIA'. Finally, the simulated yield was compared with the observed yield in the corresponding season, as well as the anthesis and crop maturity dates.

Rodríguez et al. (2010) indicate that two criteria were used to evaluate the calibration, that is, root mean standard error (RMSE) and r². The first corresponds to the square root of the mean square error RMSE = [Ó{(simulated-observed)²/N}^{0.5}], which provides the degree of dispersion between simulated and observed values, while r² provides the degree of association between simulated and observed data.

RESULTS AND DISCUSSION

Calibration of DSSAT

The calibration result of the DSSAT model was evaluated in this study using the days from planting to anthesis, total cycle duration, and final yield variables. Results allow determining an adequate calibration of DSSAT because of the proximity between simulated values and values observed in the field. For the duration of the crop development cycle datum with the adjusted coefficients (Figure 1), the model estimated a mean of 153 d from planting to maturity for 'Pandora-INIA', while it was 150 d for observed data. The estimated cycle was 154 d for 'Kipa-INIA', 12 d less than the observed mean of 170 d for this variety. Finally, the model estimated the total duration of the cycle as 170 d for 'Millán-INIA' with a mean observed value of 163 d, which is a difference of 7 d.

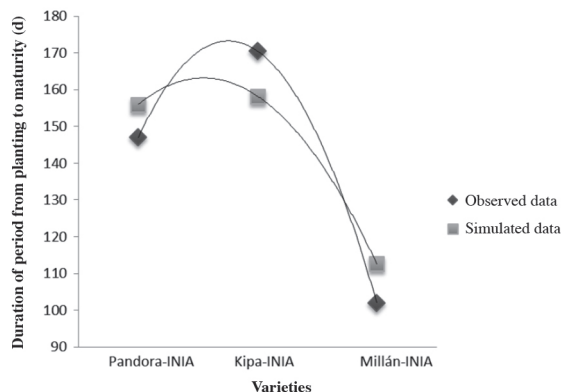


Figure 1. Comparison duration of period from planting to maturity between observed data vs. simulated data with DSSAT 4.5 of spring wheat 'Pandora-INIA', 'Kipa-INIA', and 'Millán-INIA' using adjusted genetic coefficients.

We can determine that the model adjustment is acceptable based on the RMSE values (Table 1). For the days from planting to anthesis variable, RMSE values calculated for the varieties fluctuate between 3.5 and 9.7. Other authors working with winter wheat simulations determined RMSE to be 6.6 (Rezzoug et al., 2008) and 3.0 (Bannayan et al., 2003) for this period, while our values for maturity fluctuate between 1.4 and 12.2; ranges of 7.1 (Rezzoug et al., 2008) and 10.0 (Bannayan et al., 2003) were reported.

When evaluating the degree of association between simulated and observed values for days to maturity (Table 2), 'Millán-INIA' has a very good adjustment and exhibits high r^2 and low RMSE. The other varieties exhibited low association between simulated and observed values, which shows low simulation ability for this variable that needs to be improved. Timsina and Humphreys (2006) mention that the DSSAT adjustment for phenology improves when the quantity of field data increases. It is therefore necessary to conduct new studies that improve coefficient calculation by including more detailed field information in the model that is not currently recorded, for example, number of emerged plants, date of appearance of first leaf, days from flowering to the start of grain filling, volume of water applied in each irrigation event, leaf area, number of leaves per stem at maturity, and the complete characterization of the soil profile in which the crop will be established.

Table 1. Observed and simulated values obtained with DSSAT for time periods, days from planting to anthesis, and duration of total development cycle of the wheat crop.

Variable	Observed value			Simulated value			Difference (simulated value-observed value)			RMSE		
	Pandora-INIA	Kipa-INIA	Millán-INIA	Pandora-INIA	Kipa-INIA	Millán-INIA	Pandora-INIA	Kipa-INIA	Millán-INIA	Pandora-INIA	Kipa-INIA	Millán-INIA
Days from planting to anthesis, d	90	100	102	106	107	112	+16	+7	+10	3.87	9.73	3.5
Total duration of cycle, d	150	170	163	153	154	170	+3	-12	+7	1.35	12.22	0.25

RMSE: Root mean square error.

Table 2. Coefficient of determination (r^2) and RMSE obtained from the validation of total duration of development cycle of the wheat varieties under study.

Varieties	r^2	RMSE
Pandora-INIA	0.14	1.35
Kipa-INIA	0.52	12.22
Millán-INIA	0.97	0.25

RMSE: Root mean square error.

Estimated genetic coefficients for each variety

The coefficients that are directly associated with crop phenology are P1V and P1D when soil moisture is not a limiting factor for germination and the rate of development will largely depend on the temperature *per se* (Reynolds et al., 1996). In the Mediterranean zone where this experiment was conducted, the mean temperature during the germination-emergence period was 10.6 °C in September according to the historical climate data of the Universidad de Concepción. This temperature is within the range of 2.8 to 25.0 °C required for spring wheat to germinate and emerge (Mellado, 2007), and would occur 15 d after planting with no significant differences among varieties according to field records of INIA's Wheat Breeding Program.

The results of this study show that 'Pandora-INIA', 'Millán-INIA', and 'Kipa-INIA' have the minimum requirements of vernalization. The values are represented by P1V; 'Pandora-INIA' and 'Kipa-INIA' were relatively similar, while 'Millán-INIA' showed a slightly higher value (Table 3). Given that the genotypes analyzed in this study are spring genotypes, it is logical to think that they show certain insensitivity to the vernalization processes and their requirements would be near 0 °C. However, Mellado (2007) notes that, in the case of wheat, it is not

Table 3. Estimated genetic coefficients using DSSAT GLUE for each spring wheat variety.

Varieties	Genetic coefficients estimated by DSSAT						
	P1V	P1D	P5	G1	G2	G3	PHINT
	d	%	°C d	nr g ⁻¹	mg	g	°C d
Pandora-INIA	5.00	92.00	795.00	25.00	55.00	1.00	96.00
Kipa-INIA	6.90	78.00	734.60	27.10	51.20	1.44	96.00
Millán-INIA	9.67	92.31	730.90	25.47	62.65	1.04	96.00

DSSAT: Decision support system for agrotechnology transfer, GLUE: generalized likelihood uncertainty estimation method, P1V: days with optimum temperature for vernalization, P1D: percentage reduction of development rate with a photoperiod 10 h lower than the threshold, P5: thermal time of grain filling stage), G1: number of seeds per unit canopy weight at anthesis, G2: normal seed size under optimum conditions, G3: normal dry weight (including grain) of one unstressed stem at maturity, PHINT: thermal time between appearance of successive leaves.

appropriate to assume a thermal requirement of 0 °C because this species exhibits different base and optimum temperature needs for each of its development stages. Del Pozo et al. (1987) determined that spring wheat planted in central Chile has a thermal requirement of 74 °C d for the planting to emergence period and a minimum or base temperature of 2.8 °C. This background information will allow us to determine if the calculated P1V values are within the requirement range previously reported by these authors.

The photoperiod requirement (P1D) is similar for 'Pandora-INIA' and 'Millán-INIA' and lower for 'Kipa-INIA', while thermal requirements for grain filling (P5) do not exhibit any important differences among varieties. Regarding the latter, Reynolds et al. (1996) point out that the rate of development from post-anthesis to maturity when grain filling occurs is insensitive to photoperiod and vernalization and responds positively to temperature. According to the historical database of the Universidad de Concepción, temperatures during this development period correspond to a mean of 18 °C for the Mediterranean zone where the study is conducted.

Yield and yield components

Two important yield components are the number and weight of seeds represented by coefficients G1 and G2. These components show differences among varieties and there exists a compensatory effect since decreasing G1 increases G2. This negative relationship could be explained by the fact that the number of available assimilates for filling decreases when the number of grains m⁻² increases; their individual weight would be reduced because of the competition that is generated among them (Reynolds et al., 1996). The G3 coefficient did not show any high variations among varieties. This factor would be related to biomass production and plant height. Given that these varieties have a mean height of 90 cm and a harvest index of 0.45, the similarity of thermal requirements for G3 could be explained.

The planting to emergence stage is followed by the vegetative stage with the appearance of leaves around the main stem; this process is also known as phyllochron (PHINT). Rickman and Klepper (1991) indicate that this stage is highly dependent on temperature. The three varieties in this analysis require 96 °C d to carry out this process, which is related to what happens in the field and because these varieties do not exhibit significant differences in the duration of the vegetative stage, that is, 86 d for 'Pandora-INIA' (Mellado and Madariaga, 2003), 90 to 95 d for 'Kipa-INIA' (Matus et al., 2011a), and 88 to 89 d for 'Millán-INIA' (Matus et al., 2011b).

Once all the leaves have appeared on the main stem, flowering occurs (McMaster et al., 2008), which is strongly determined by vernalization (P1V) and photoperiod (P1D) (Brooking, 1996; Mahfoozi et al., 2001; Brooking and Jamieson, 2002). Photoperiod defines floral initiation

(Hoogenboom et al., 2003) and grain filling (P5), stage which is highly influenced by the environment as are previous stages (Wheeler et al., 1996).

According to the results (Table 3), the coefficients of 'Pandora-INIA' and 'Millán-INIA' do not exhibit any significant differences. However, the 'Kipa-INIA' variety shows a significantly lower requirement for P1D and P5. This is important given that Matus et al. (2011a) mention that the spike appears 90 to 95 d after planting; this would suggest that its complete development cycle exceeds that of the other two varieties. Nevertheless, its growth period ranges from 150 to 170 d just like 'Pandora-INIA' and 'Millán-INIA'; this would allow us to assume that, because of its lower P1D and P5 requirements, 'Kipa-INIA' grain filling could be done over a shorter time and thus complete its development in a time period similar to the other two varieties. Mellado (2007) shows that when considering the whole life cycle of the wheat plant and base temperature, mean thermal requirement reaches 1400 °C d. However, this value is affected by climate where the duration of the phenological period is lower when air temperature is higher.

Validation of the model

An independent dataset was used to evaluate and validate the model, which was not the same one used to calibrate the genetic coefficients. Figure 2 displays the result with adjusted coefficients for 'Pandora-INIA', 'Kipa-INIA', and 'Millán-INIA' by comparing simulated and observed yields (Mg ha⁻¹). Coefficients of correlation for yield were r²: 0.78 for 'Pandora-INIA', 0.72 for 'Kipa-INIA', and 0.81 for 'Millán-INIA', and the RMSE values were considered low for the three varieties (Table 4); this indicates that the model simulates quite closely to real yields for each variety. However, RMSE for 'Pandora-INIA' is significantly higher, indicating a greater data dispersion of data and, therefore, more field information and greater calibration work would be needed to decrease the error of estimate. Even so, the r² and RMSE statistics

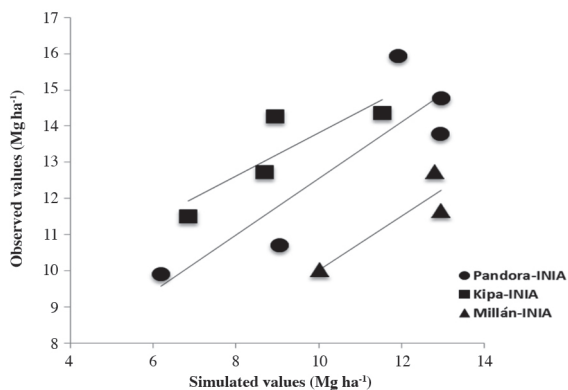


Figure 2. Observed vs. simulated yields with DSSAT 4.5 of spring wheat 'Pandora-INIA', 'Kipa-INIA', and 'Millán-INIA' using adjusted genetic coefficients.

Table 4. Coefficient of determination (r^2) and RMSE obtained from the validation for yield of the wheat varieties under study.

Varieties	r^2	RMSE (kg ha ⁻¹)
Pandora-INIA	0.78	1117.29
Kipa-INIA	0.72	626.73
Millán-INIA	0.81	406.46

RMSE: Root mean square error.

corresponding to each variety emphasize that the procedure used to calculate the genetic coefficients was adequate by simulating fairly closely the yields in the location under study.

Finally, the development and adaptation of this type of tools in the process of generating new wheat varieties will allow greater efficiency in the adaptation process of the new scenarios generated by climate change on agriculture, and allow the evaluation of different productive conditions once the genetic coefficients of the varieties are obtained.

CONCLUSIONS

The calibration and validation of the DSSAT model for the three spring bread wheat varieties under Mediterranean climate conditions was highly efficient in predicting their yield.

Regarding quality estimation of the phenological traits, there was a minor precision attributed to the need for more detailed agronomic information (number of emerged plants, date of appearance of first leaf, days from flowering to the start of grain filling, volume of water applied in each irrigation event, leaf area, and number of leaves per stem at maturity).

ACKNOWLEDGEMENTS

Research was conducted thanks to contributions from the FONTAGRO Project: “Variabilidad y Cambio Climático en la Expansión de la Frontera Agrícola en el Cono Sur: Estrategias Tecnológicas para Reducir Vulnerabilidades”, FTG-8011/08.

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