

**University of São Paulo
“Luiz de Queiroz” College of Agriculture**

**Calibration, uncertainties and use of soybean crop simulation models for
evaluating strategies to mitigate the effects of climate change in
Southern Brazil**

Rafael Battisti

Thesis presented to obtain the degree of Doctor in
Science. Area: Agricultural Systems Engineering

**Piracicaba
2016**

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RESUMO

Calibração, incertezas e uso de modelos de simulação da soja para avaliar estratégias de mitigação aos efeitos das mudanças climáticas na região Centro-Sul do Brasil

O déficit hídrico é o principal fator causador de perda de produtividade para a soja no Centro-Sul do Brasil e tende a aumentar com as mudanças climáticas. Alternativas de mitigação podem ser avaliadas usando modelos de simulação de cultura, os quais diferem em nível de complexidade e desempenho. Baseado nisso, os objetivos desse estudo foram: avaliar cinco modelos de simulação para a soja e a média desses modelos; avaliar a sensibilidade dos modelos a mudança sistemática do clima; avaliar características adaptativas da soja ao déficit hídrico para o clima atual e futuro; e avaliar a resposta produtiva de manejos da soja para o clima atual e futuro. Os modelos utilizados foram FAO – Zona Agroecológica, AQUACROP, DSSAT CSM-CROPGRO-Soybean, APSIM Soybean e MONICA. Os modelos foram calibrados a partir de dados experimentais obtidos na safra 2013/2014 em diferentes locais e datas de semeadura sob condições irrigadas e de sequeiro. Na análise de sensibilidade foram modificadas a temperatura do ar, [CO₂], chuva e radiação solar. Para as características de tolerância ao déficit hídrico foram manipulados, apenas no modelo DSSAT CSM-CROPGRO-Soybean, a distribuição do sistema radicular, biomassa divergida para crescimento radicular sob déficit hídrico, redução antecipada da transpiração, limitação da transpiração em função do déficit de pressão de vapor, fixação de N₂ sob déficit hídrico e redução da aceleração do ciclo devido ao déficit hídrico. Os manejos avaliados foram irrigação, data de semeadura, ciclo de cultivar e densidade de semeadura. A produtividade estimada obteve raiz do erro médio quadrático (REMQ) variando entre 553 kg ha⁻¹ e 650 kg ha⁻¹, com índice d acima de 0.90 para todos os modelos. O melhor desempenho foi obtido utilizando a média de todos os modelos, com REMQ de 262 kg ha⁻¹. Os modelos obtiveram diferentes níveis de sensibilidade aos cenários climáticos, reduzindo a produtividade com aumento da temperatura, maior taxa de redução da produtividade com menor quantidade de chuva do que aumento de produtividade com maior quantidade de chuva, diferentes respostas com a mudança da radiação solar em função do clima local e do modelo, e resposta positiva assintótica para o aumento da concentração de [CO₂]. Quando combinado as mudanças dos cenários, a produtividade foi afetada principalmente pela redução da chuva (aumento da radiação solar), enquanto a mudança na temperatura e [CO₂] mostrou compensação nas perdas e ganhos. A distribuição do sistema radicular foi o mecanismo de tolerância ao déficit hídrico com maior ganho de produtividade, representando ganho total na produção de 3,3 % e 4,0% para a região, respectivamente, para o clima atual e futuro. Para os manejos não se observou melhores resultados com a mudança do manejo para o futuro em relação a melhor condição para o clima atual. Desta forma, os modelos mostraram diferentes desempenho, em que a parametrização e a estrutura do modelo afetaram a resposta das alternativas avaliadas para mudanças climáticas. Apesar das incertezas, os modelos de cultura são uma importante ferramenta para avaliar o impacto e alternativas de mitigação as mudanças climáticas.

Palavras-chave: *Glycine max* L.; Comparação de modelos; Média de modelos; Cenários de clima futuro; Adaptação à seca; Manejo de cultura

ABSTRACT

Calibration, uncertainties and use of soybean crop simulation models for evaluating strategies to mitigate the effects of climate change in Southern Brazil

The water deficit is a major factor responsible for the soybean yield gap in Southern Brazil and tends to increase under climate change. Crop models are a tool that differ on levels of complexity and performance and can be used to evaluate strategies to manage crops, according the climate conditions. Based on that, the aims of this study were: to assess five soybean crop models and their ensemble; to evaluate the sensitivity of these models to systematic changes in climate; to assess soybean adaptive traits to water deficit for current and future climate; and to evaluate how the crop management contribute to soybean yields under current and future climates. The crop models FAO - Agroecological Zone, AQUACROP, DSSAT CSM-CROPGRO-Soybean, APSIM Soybean, and MONICA were assessed. These crop models were calibrated using experimental data obtained during 2013/2014 growing season in different sites, sowing dates and crop conditions (rainfed and irrigated). For the sensitivity analysis was considered climate changes on air temperature, [CO₂], rainfall and solar radiation. For adapting traits to drought, the soybean traits manipulated only in DSSAT CSM-CROPGRO-Soybean were deeper root depth, maximum fraction of shoot dry matter diverted to root growth under water stress, early reduction of transpiration, transpiration limited as a function of vapor pressure deficit, N₂ fixation drought tolerance and reduced acceleration of grain filling period in response to water deficit. The crop management options strategies evaluated were irrigation, sowing date, cultivar maturity group and planting density. The estimated yield had root mean square error (RMSE) varying between 553 kg ha⁻¹ and 650 kg ha⁻¹, with d indices always higher than 0.90 for all models. The best performance was obtained when an ensemble of all models was considered, reducing yield RMSE to 262 kg ha⁻¹. The crop models had different sensitivity level for climate scenario, reduction yield with temperature increase, higher rate of reduction of yield with lower rainfall than increase of yield with higher rainfall amount, different yields response with solar radiation changes due to baseline climate and model, and an asymptotic soybean response to increase of [CO₂]. Combining the climate scenarios, the yield was affected mainly by reduction of rainfall (increase of solar radiation), while temperature and [CO₂] interaction showed compensation effect on yield losses and gains. The trait deeper rooting profile had greater improvement in total production for the Southern Brazil, with increase of 3.3 % and 4.0 %, respectively, for the current and future climates. For soybean management, in most cases, the models showed that no crop management strategy has a clear tendency to result in better yields in the future if shift from the best management of current climate. This way, the crop models showed different performance against observed data, where the model parametrization and structure affected the response to alternatives managements to climate change. Although these uncertainties, crop models and their ensemble are an important tool to evaluate impact of climate change and alternatives to mitigation.

Keywords: *Glycine max* L.; Models comparison; Models ensemble; Future climate scenarios; Adaptation to drought; Crop management

1 INTRODUCTION

The soybean grain can be used to produce several types of products, such as refined oil for cooking, biodiesel, defatted flour, meal to animal feeding, isolated protein, and, also, as fresh food (EMBRAPA, 2015). Due to these varieties of products and sub-products, soybean is a crop of major importance around the world, being the fourth in cropped area (FAO, 2016). Among the countries that produce soybean, Brazil was responsible for approximately 30% of the global production in 2013 (FAO, 2016). In the 2014/2015 growing season, Brazil had a total soybean area of 32.09 million hectares, with total production of 96.23 million tons, resulting in an average yield of about 3000 kg ha⁻¹ (COMPANHIA NACIONAL DE ABASTECIMENTO - CONAB, 2016). Southern Brazil (Figure 1), which includes five states, is responsible for almost 45% of Brazilian soybean production in 2015 (CONAB, 2016).

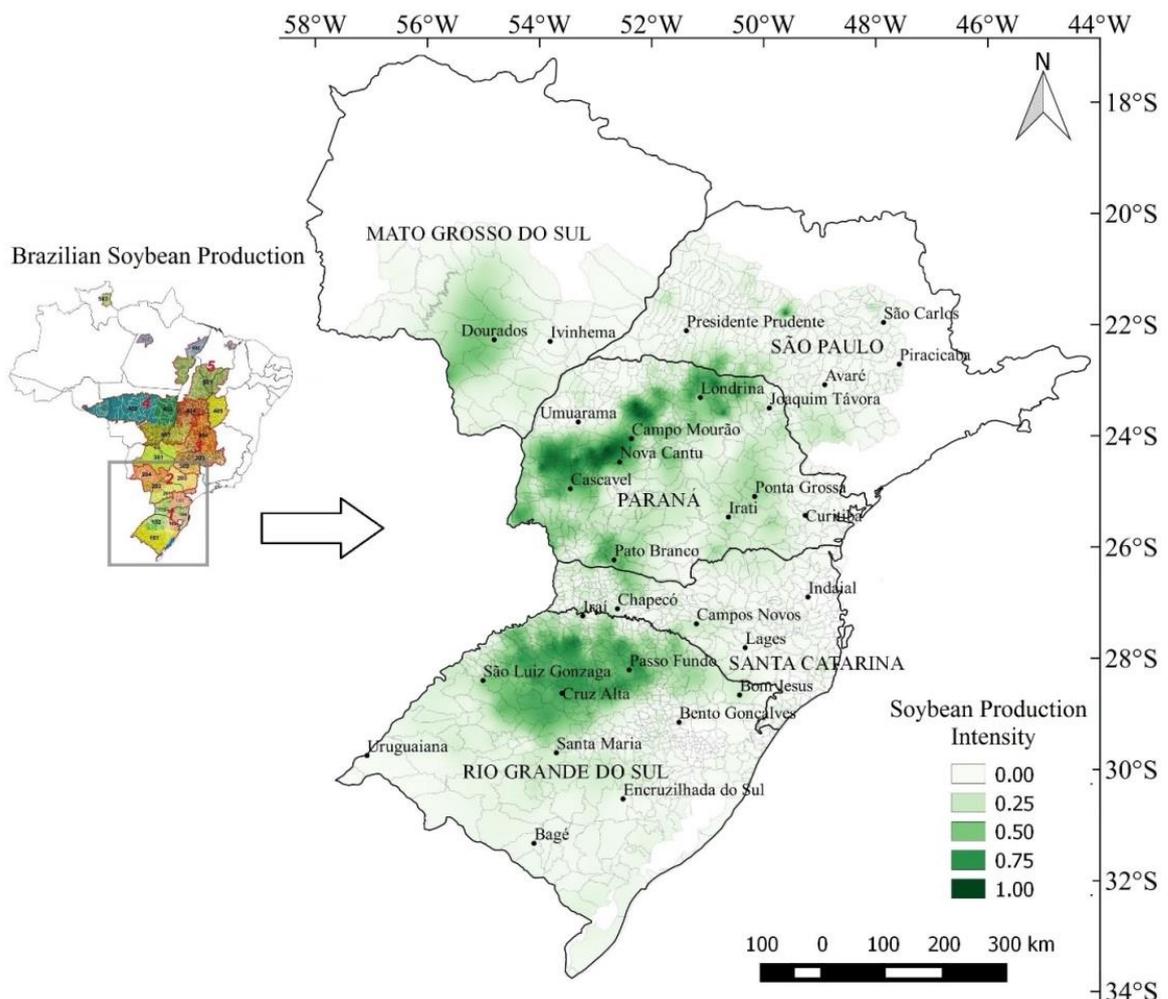


Figure 1 – Soybean crop distribution in Southern Brazil. The values in the legend represent the decimal part of a pixel cultivated with soybean. Adapted from Instituto Brasileiro de Geografia e Estatística - IBGE (2015)

Soybean yield is highly influenced by environmental conditions, mainly by weather conditions. In Brazil, the main environmental factor responsible for yield losses in rainfed soybean is drought, which is responsible for approximately 74% of yield gap, reducing yields, in average, by 30% (SENTELHAS et al., 2015). The Brazilian soybean yield is also affected by rainfall interannual and intraseasonal variability, which differ between producing regions (SENTELHAS; BATTISTI, 2015) (Figure 2). In Southern Brazil, the soybean yield variability is higher than other regions (BERLATO et al., 2005), which is mainly due to the effects of the phenomenon El Niño Southern Oscillation (ENOS), which has stronger influences in this region than in other parts of Brazil (BERLATO; FONTANA, 2003). Normally, a reduction in rainfall is observed during La Niña phase (Figure 2b), whereas an increase occurs during El Niño phase (FARIAS et al., 2007). Such climate variability tends to become more frequent under climate change scenarios, mainly in the tropical and subtropical regions (LI et al., 2013), although the high uncertainties associated to rainfall future projections for Southern Brazil (MARENGO et al., 2010; CHOU et al., 2012).

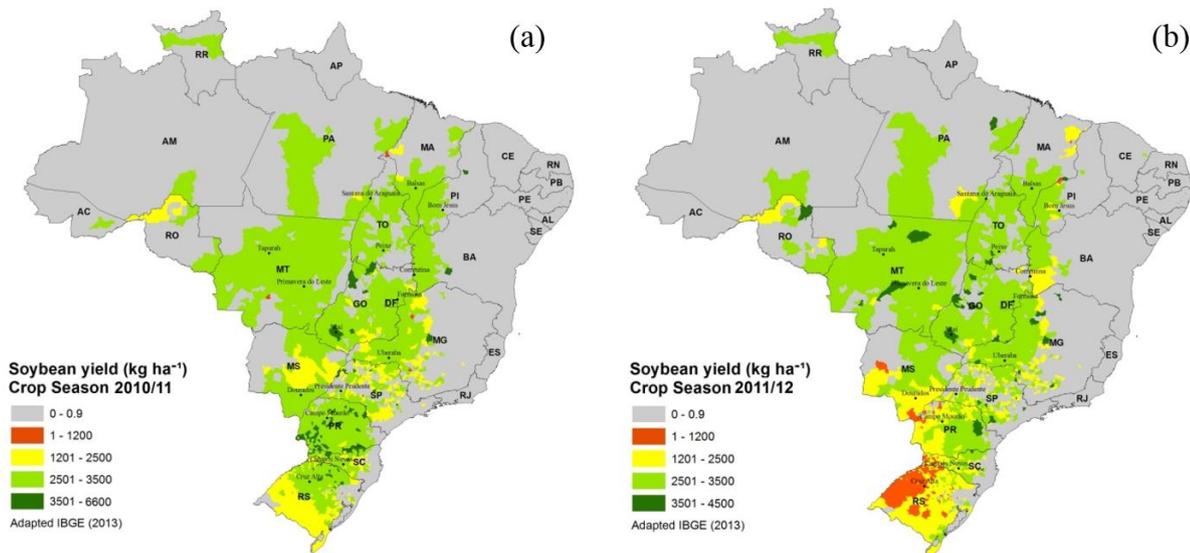


Figure 2 – Soybean yield in the crop seasons of 2010/11 (neutral year) (a) and 2011/12 (La Niña year) (b), in Brazil

The air temperature and photoperiod affect soybean development, altering the interaction between the crop phases and weather conditions, and, consequently, soybean yield (FIETZ; RANGEL, 2008). For example, if water deficit occurs during grain filling, the yield losses will be greater than if it occurs during vegetative phase (DOGAN et al., 2007; BATTISTI; SENTELHAS, 2015). The air temperature also affects the photosynthesis rate, due to the balance between gross photosynthesis and maintenance respiration, defining the

photoassimilates available to crop growth (PEREIRA et al., 2002). The most suitable range of temperature for soybean crop is between 20 and 30°C (FARIAS et al., 2009), although higher gross photosynthesis can be observed till 40°C (BOOTE et al., 1998). Extreme values also affect soybean, reducing development and growth. Air temperatures below 20°C and above 55°C during initial phases reduce the development of initial phases, whereas during vegetative phase air temperatures below 10°C result in null crop growth, and above 40°C there is reduction of pod number (NEUMAIER et al., 2000; FARIAS et al., 2009).

Solar radiation provides energy for photosynthesis and environmental signals to several physiological processes in soybean, which associated with air temperature, defines the potential yield (SENTELHAS et al., 2015). In Brazil, there is no solar radiation limitation for soybean production, which is mainly caused by the geographic position of the country, between 5° North and 30° South. However, in some locations, the intense presence of clouds results in lower soybean potential yield. Casaroli et al. (2007) observed that soybean radiation use efficiency reached 1.2 grams of dry matter by MJ of photosynthetic active radiation intercepted, although this can vary between cultivars (GILBERT et al., 2011; BARONIYA et al., 2014). The photosynthesis also is affected by [CO₂], which actually is close to 400 ppm (INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE - IPCC, 2014). For soybean, the yield can be improved if [CO₂] increase, since C₃ plants in the current [CO₂] have not rubisco enzyme saturated (WALTER et al., 2015).

For the future climate, there is a clear trend of increasing air temperature and [CO₂] in the atmosphere, with possible changes, also, in the amount and distribution of rainfall and, consequently, in the availability of solar radiation (IPCC, 2014). The increase in air temperature will result in a higher crop transpiration, which will possibly lead to more water deficit for crops. On the other hand, the increase of [CO₂] can improve water use efficiency, due to photosynthesis increase and stomata conductance reduction (WULLSCHLEGER et al., 2002). The responses of soybean crop to [CO₂] and air temperature increases are directly related with soil water availability for the plants, as observed by Li et al. (2013). According to these authors, soybean yield will improve with the increase of [CO₂] only if soil was well-watered. Deryng et al. (2014) observed that [CO₂] increase can compensate yield losses due to higher air temperature for soybean depending on the current climate. In general, it is expected that the crops looking for adapting to rising CO₂, heat stress, and water deficit, will increase their efficiency for water and nutrients use (WHITE et al., 2011).

In this context, it is important to evaluate how will be the crops responses to climate change in a specific regions (LEHMANN et al., 2013), and which are the strategies that can

be adopted to reduce the negative impacts of climate change on yields (MATTHEWS et al., 2013). Both evaluations can be done by using crop simulation models, which allow to manipulate genetic traits, climate and crop management, and see how the combination of them will affect yields. However, crop simulation models differ in the way and level they simulate dynamic processes, which is associated to the uncertainties in the models' parameters and structure (PALOSUO et al., 2011; ASSENG et al., 2013; BASSU et al., 2014; MARTRE et al., 2015).

One of the advantages of using crop simulation models is the possibility of extrapolation of the simulations from a single year or a single experimental site to different sites and climate conditions (JONES et al., 2003). This extrapolation is important because it is not possible to have conclusive results about management strategies based on a single field experiment (EGLI; CORNELIUS, 2009). Despite this advantage, the field experiments are essential for crop models calibration and evaluation (HUNT; BOOTE, 1998).

The differences in structure and parametrization between distinct crop simulation models are leading to the development of studies that compare the models' performance under different environmental conditions. These comparisons are performed to reduce the uncertainties in the predictions through the model improvement (PORTER et al., 1993; JAMIESON et al., 1998), and/or to analyze the results from simulations based on multi-models ensembles (PALOSUO et al., 2011; ASSENG et al., 2013). The crop models also are being evaluated under climate change scenarios, by using systematic changes in climate variables (sensitivity analysis), which help to understand the model performance under different climate conditions and to identify the limitations of them. These type of analyses were performed for wheat (ASSENG et al., 2013; MARTRE et al., 2015; PIRTIOJA et al., 2015), maize (BASSU et al., 2014; ARAYA et al., 2015), rice (LI et al., 2015) and sugarcane (MARIN et al., 2015), while for soybean this kind of study is still restricted (WHITE et al., 2011).

The crop models can be used for many purposes, given support for choosing the best management strategies under different environmental conditions (WHITE et al., 2011). Among the possibility of uses, the crop models can be applied to determine the best sowing dates (DALLACORT et al., 2008; BATTISTI; SENTELHAS, 2014), drought tolerance traits (SINCLAIR et al., 2010; BOOTE, 2011), irrigation management (DOGAN et al., 2007), best cultivars and maturity groups (BOOTE et al., 2003; BAO et al., 2015) and climate change effects on yields (WHITE et al., 2011; ASSENG et al., 2013; ALAGARSWAMY et al., 2006; NENDEL et al., 2009). It is important to mention that in this type of analysis there is no

“error free” model or “best” model performance, which requires a careful evaluation of the results (PALOSUO et al., 2011).

Once crop models calibration and evaluation for a given locations are concluded, they can be used to evaluated different strategies for climate change impacts mitigation, in order to improve yield. Ewert et al. (2015) observed that changes of sowing dates, together with changes in cropping systems, such as cultivars and crop rotation, are the most evaluated management strategies to increase crop resilience in relation to climate change. These authors also mentioned that new practices, such as fertilization and tillage, interaction practices, as planting dates and irrigation, and improvement of crop characteristics are still marginally investigated. Based on that, the mitigation strategies can follow two ways (MATTHEWS et al., 2013): the adaptation based on breeding programs through the introduction of new cultivars with higher drought tolerance (SINCLAIR et al., 2010) and the use of crop management strategies to reduce the yield gap, such as use of supplementary irrigation (NENDEL et al., 2014), adoption of new sowing dates (DO RIO et al., 2015), maturity groups (KUMAGAI; SAMESHIMA, 2014) and plant densities (VAZQUEZ et al., 2014), as well as theirs interactions for both current and future climates.

For breeding programs, a better cultivar can be developed by adjusting their morphological and physiological functions for adapting the crop to the environment (GILBERT et al., 2011). The adaptation to water deficit and high temperatures can be done by evaluating soybean traits in new cultivars in order to improve yield and reduce the yield gap for the current and future climates (BOOTE, 2011). The first step to mitigate yield losses is to identify soybean breeding lines with advantageous traits that can help the crop to adapt to adverse conditions, such as water deficit (LEHMANN et al., 2013). Cultivars characteristics, such as deeper and denser root system (BORTOLUZZI et al., 2014), soil water conservation (SINCLAIR et al. 2008; GILBERT et al., 2011), nitrogen fixation drought tolerance (SINCLAIR et al., 2007), and less sensitivity of grain filling acceleration under drought (SPECHT et al., 1986) have potential to be used to develop new cultivars, more resilience to water deficit.

On the other hand, the crop management can improve yields. Irrigation, when possible, is a strategy that results in yield stability between crops seasons (NENDEL et al., 2014). The irrigation has interactions with other crop management strategies, such as plant density (KUSS et al., 2008), and also with climate conditions, as [CO₂] (LI et al., 2013). Changes of sowing dates and cultivar maturity groups can be strategically used to avoid heat and drought stresses (BAO et al., 2015), whereas crop cycle interacting with climate

conditions, can reduce the yield losses caused by water deficit. According to Kassie et al. (2015), in a humid climate under current or future scenario, a medium cycle cultivar has significant higher yield than a short cycle cultivar.

Based on the importance of soybean crop for feeding the world population and the contribution of Southern Brazil in the global market, it is essential to assess the effect of climate change on this crop and the alternatives to mitigate the negative impacts in this region in order to improve crop yield. The hypotheses of this study are that crop models had different performance to predict yield under current and future climate conditions, requiring calibration and evaluation for the specific regions, and that crop models can be used efficiently to assess alternatives to improve the crop resilience and, consequently, the soybean yield in different climate conditions. Therefore, this study had the following general and specific objectives:

1.1 Objectives

1.1.1 General

The general objective of this study was to assess the soybean yield and alternative strategies to mitigate the negative effect of climate change on that and to improve soybean yield based on the current and future climates using an ensemble of five crop simulation models in Southern Brazil.

1.1.2 Specific

- a) to calibrate and evaluate the following soybean crop simulation models: FAO – Agroecological Zone; FAO – AQUACROP; Model for Nitrogen and Carbon in Agroecosystems (MONICA); Crop Simulation Model – CROPGRO – Soybean (CSM-CROGGRO-Soybean); and Agricultural Production Systems Simulator (APSIM);
- b) to perform a sensitivity analysis of the crop models to simulate soybean growth and development under systematic changes of air temperature, [CO₂], rain and solar radiation;
- c) to assess yield response for different soybean traits to improve drought tolerance by using the Crop Simulation Model – CROPGRO – Soybean (CSM-CROGGRO-Soybean);

d) to evaluate the soybean yield response to the following crop management strategies: irrigation; sowing dates; cultivars maturity groups; and plant densities simulated by an ensemble of the crop models for current and future climate scenarios.

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2 INTER-COMPARISON OF FIVE SOYBEAN CROP SIMULATION MODELS AND THEIR ENSEMBLE

Abstract

Crop simulation models can help scientists, government agencies and growers to evaluate the best strategies to manage their crops in the field, according the climate conditions. Currently, there are many crop models available to simulate soybean growth, development, and yield, with different levels of complexity and performance. Based on that, the aim of this study was to assess five soybean crop models and their ensemble in Southern Brazil. The following crop models were assessed: FAO - Agroecological Zone; AQUACROP; DSSAT CSM-CROPGRO- Soybean; APSIM Soybean; and MONICA. These crop models were calibrated using experimental data obtained during 2013/2014 growing season in different sites, sowing dates and crop conditions (rainfed and irrigated) for cultivar BRS 284, totaling 17 treatments. The crop variables assessed were: grain yield; crop phases; harvest index; total above-ground biomass; and leaf area index. The calibration was made in three levels: using original coefficients from models' default (no calibration); calibrating the coefficients related only with crop development; and calibrating all set of coefficients (crop development, growth, and soil conditions). The results from the models were analyzed individually and in an ensemble of them. The crop models showed an improvement of performance from no calibration to complete calibration. Crop phases were estimated efficiently, although different approaches were used by the models. The estimated yield had RMSE varying between 535 kg ha⁻¹ for MONICA and 650 kg ha⁻¹ for FAO models, with d indices always higher than 0.90 for all of them. The best performance was obtained when an ensemble of all models was considered, reducing yield RMSE to 262 kg ha⁻¹. The same tendency was observed for leaf area index. The harvest index was the crop variable with the poorest performance. In a general way, the results showed that an ensemble of completely calibrated models were more efficient to simulate soybean yield than any single one

Keywords: Model calibration; Model evaluation; Models' ensemble; FAO - Agroecological Zone; AQUACROP; DSSAT; APSIM; MONICA

2.1 Introduction

The soybean is a major crop around of world, being source of oil (refined for cooking and biodiesel production), defatted soy flour, soybean meal (animal feeding), isolated protein, and as fresh food used for cooking (EMBRAPA, 2015). Due to its multiple uses, soybean is the largest crop grown in Brazil, with 30.9 million hectare in the 2014/2015 crop season (CONAB, 2015), while it is the fourth largest crop cultivated in the world, with 111.3 million hectare in 2013 (FAO, 2015).

Soybean grain demand is increasing constantly as a function of population growth, thus it is necessary to improve production, mainly by yield increase, in a sustainable way (SENTELHAS et al., 2015). In this context, crop models can help in the assessment of the

best strategies to achieve this goal, provided they are able to evaluate the best sowing dates (BATTISTI; SENTELHAS, 2014), the effects of climate change on yield (WHITE et al., 2011; ASSENG et al., 2013), identify drought tolerance traits (SINCLAIR et al., 2010; BOOTE, 2011), as well as many other possibilities (TSUJI et al., 1998; WALLACH et al., 2006).

Different crop models have been developed and evaluated for soybean crop using data from specific regions and field scales. Beyond of parametrization from these regions, these crop models differ in the way and level that they simulate dynamic processes, as water balance and crop growth and development (WHITE et al., 2011), creating uncertainties related to the model's parameters and structure (PALOSUO et al., 2011). It is important to highlight that the level of model complexity is not related with accuracy of results (SENTELHAS, 2011), once well calibrated simple models can be as accurate as the complex ones. Zhang et al. (2002) showed that the total error of a model's prediction is the sum of systematic and calibration errors, and when a simple model is used, the total error is mainly caused by systematic error. Otherwise, when the complexity of model is increased, including new processes of simulation, the systematic error tend to be reduced, but calibration error increases, once many coefficients requires calibration.

The applicability of a crop model is related with the level of interactions and processes included in the model. For example, the FAO-Agroecological zone model is a simple crop model used to evaluate the relationship between crop yield and climate conditions (DOORENBOS; KASSAM, 1979). Battisti and Sentelhas (2015) observed that this model was able to estimate soybean yield efficiently in Brazil, even considering its simplicity. According to Jamieson et al. (1998), the reason for the good performance of simple crop models to estimate yield is because there are accurate models to simulate crop evapotranspiration and water balance, once water deficit is the main yield factor for the majority of rainfed crops.

On the other hand, complex crop models have more details in the description of all crop processes, which increase the number of possible uses of them to evaluate crop development and yield, and the influence of crop management on these variables. For example, CROPGRO model integrates carbon, nitrogen and water balances on growth processes (BOOTE et al., 2003). These characteristics associated with other important processes, as the relationship between photosynthesis and [CO₂], make the models able to simulate soybean yield for several conditions, including under future climate scenarios (BOOTE et al., 1997; ALAGARSWAMY et al., 2006). Under this point of view, it is

important to know the level of interaction between different processes on the crop models, identifying limiting points and possibilities of simulations with each one.

The huge variety of crop models' structures and parametrizations are leading for the development of studies that compare their performance under different conditions (PORTER et al., 1993; JAMIESON et al., 1998). Complimentary, these models can also be used for multi-models ensembles (PALOSUO et al., 2011; ASSENG et al., 2013), in order to improve the accuracy and reduce the uncertainties (ASSENG et al., 2013), once there is no "error free" or "best" model performance (PALOSUO et al., 2011).

In a global level, the Agricultural Model Intercomparison and Improvement Project - AGMIP (www.agmip.org) has developed studies to compare crop models, aiming to improve crop and economic models for enhance projections of future food production, evaluating the effect of climate change and adaptation measures on crop yields and food prices (ROSENZWEIG et al., 2013). The group proposed that crop models improvement needs to be related with CO₂, temperature and water interactions and accounting for yield gaps due to water, nitrogen, pest, diseases and other factors.

Based on that, we believe that multiple-models ensemble can reduce the uncertainties in the crop yield simulations. Therefore, the aims of this study were: to calibrate five crop simulation models for soybean crop based on crop growth and development under different water levels from field experiments conducted in Southern Brazil; to evaluate the crop models performance using different levels of calibration and models ensemble approach; and to define the limiting points and the main steps in calibration process for each one of the crop models.

2.2 Materials and Methods

2.2.1 Field experiments

The soybean development, growth and yield data were obtained from two sets of field experiments, where the first set was used for the crop model calibration and the second for the model evaluation (Table 1). The first experiment was carried out during 2013/14 crop season in three locations in Southern Brazil: Frederico Westphalen, RS, Londrina, PR, and Piracicaba, SP. The second set of experiments was conducted in 2014/15 crop season in Frederico Westphalen and Piracicaba. More details about field experiment are presented in Appendix A. In addition, for model evaluation, yield data from cultivar tests in five locations

in the state of Mato Grosso do Sul, obtained from Fundação MS (2015), were also used (Table 1), considering the following locations: Dourados; Naviraí; São Gabriel do Oeste; Antônio João; and Maracajú. Details about site locations, sowing dates and crop water management are shown in Table 1, while Figure 1 is shown the geographic position of each site and their respective Köppen's climate classification, according to Alvares et al. (2013). Details about climate variability, as air temperature, solar radiation, rainfall, irrigation and potential and actual evapotranspiration during field experiments are showed in the Annex A.

Table 1 – Location, crop season, sowing dates and water management for the experimental data used for crop models calibration and evaluation

Location	Crop Season	Sowing dates	Water management
Calibration			
Frederico Westphalen, RS; 27° 21'S, 53° 23'W, 522 m ASL	2013/14	01/Oct, 18/Oct, 08/Nov, 25/Nov and 15/Dec	Rainfed
Londrina, PR; -23° 18'S, 51° 09'W, 585 m ASL	2013/14	10/Oct, 31/Oct, and 19/Nov	Rainfed and Partial Irrigation
Piracicaba, SP, 22° 43'S, 47° 38'W, 547 m ASL	2013/14	18/Oct, 14/Nov, and 08/Jan	Rainfed and Full Irrigation
Evaluation			
Frederico Westphalen, RS; 27° 21'S, 53° 23'W, 522 m ASL	2014/15	21/Oct, 19/Nov and 18/Dec	
Piracicaba, SP, 22° 43'S, 47° 38'W, 547 m ASL	2014/15	29/Nov, 08/Dec and 22/Dec	
Dourados, MS, 22° 13'S, 54° 48'W, 430 m ASL	2013/14	19/Oct and 31/Oct	
Naviraí, MS, 23° 03'S, 54° 11'W, 362 m ASL	2013/14	09/Oct and 18/Oct	Rainfed
São Gabriel do Oeste, MS, 19° 23'S, 54° 33'W, 658 m ASL	2013/14	14/Oct and 25/Oct	
Antônio João, MS, 22° 11'S, 55° 56'W, 681 m ASL	2014/15	20/Oct	
Maracajú, MS, 22° 11'S, 55° 56'W, 681 m ASL	2013/14	29/Oct	
Maracajú, MS, 21° 36'S, 55° 10'W, 384 m ASL	2013/14	26/Sept, 11/Oct and 21/Oct	
	2014/15	04/Nov	

The cultivar used in all field trials was BRS 284, maturity group 6.5, indeterminate growth habit, and a conventional material. This cultivar was chosen since it is recommended for the region of this study and for having a high potential yield. In the field experiment, fertilization was applied to sustain crop growth without deficiency and was performed according to soil analysis, by applying mainly P and K and using rhizobium inoculation to improve soybean N fixation. The crop management followed EMBRAPA's recommendations, keeping the crop free of pests and diseases (EMBRAPA, 2013). The only

exception was observed in 2014/2015 crop season in Frederico Westphalen and Piracicaba, where high Asian soybean rust severity reduced the yields, even with intensive chemical control. The spacing between rows was between 0.45 and 0.50 m, with the plant population between 26 and 32 plants m^{-2} , respectively for highest and lowest latitudes (EMBRAPA, 2013). In the most of locations the soybean was cultivated in no-tillage crop system, except for the experiment in Piracicaba, in 2013/2014 crop season, where conventional tillage system was used. During 2013/2014 crop season, the field experiments in Piracicaba had a full irrigation, while in Londrina the irrigation supplied around 75% of crop evapotranspiration. For the other experimental sites, irrigation was used only after sowing to guarantee the emergence when required. The total irrigation applied in each site is presented in the Annex A.

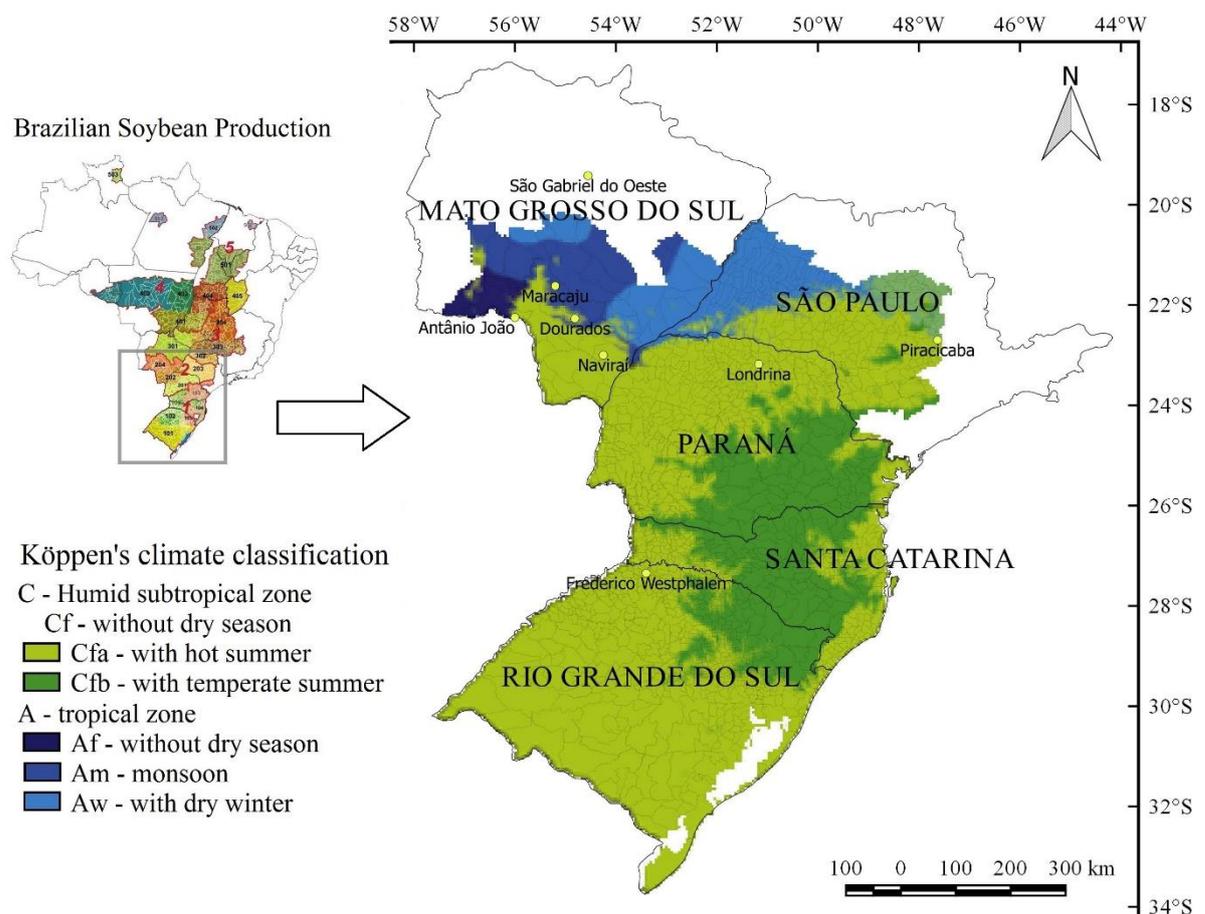


Figure 1 – Soybean field experiments in southern Brazil used in the present study and their respective Köppen's climate classification. Adapted from Alvares et al. (2013)

2.2.2 Weather and soil data

Soil characteristics and weather data are the main inputs from field experiment in the crop models, as well as information about crop management such as sowing date, irrigation, row spacing, plant population and cultivar, as previously described. For Piracicaba, Londrina and Frederico Westphalen, the weather data were obtained from National Meteorological Institute weather stations located near each experiment (± 100 m), while for the sites where the test of cultivars were performed, the weather data were also obtained from stations of the National Meteorological Institute, but considering those that were in the same municipality. The following daily weather data were used: maximum and minimum air temperature; relative humidity; wind speed at 2 m; incoming solar radiation; and rainfall.

The soil data used to build soil profile for each crop model are presented in Annex B and Appendix B. For FAO model, only total soil water holding capacity for the crop was considered. For MONICA model, the type of soil was defined based on the clay, silt and sand content and on the model's soil database. For APSIM, DSSAT and AQUACROP, the soil profiles were created based on the curve number that defines water infiltration (SOIL CONSERVATION SERVICE, 1972), bulk density, soil saturation, drained upper limit, lower limit and saturated conductivity. Soil analysis was limited to 0.50 m, which required extrapolations to the maximum root depth, with each model presenting a different definition for that (PALOSUO et al., 2011). As maximum root depth varies according each one of these models, it was one of the parameters adjusted during the calibration process.

The soils from the sites where the test of cultivars were defined based on the main soil type from the IBGE (2015) soil map. According to that, Ferralsol (Latossolo Vermelho) was defined as the main soil for all sites. After that, data from RADAMBRASIL (1974) was used to define the clay (66%), silt (19%) and sand (16%) content on this soil type. Based on these information, pedotransfer functions from Lopes-Assad et al. (2001) and Reichert et al. (2009) were used to estimate the soil water content at wilting point ($0.22 \text{ cm}^3 \text{ cm}^{-3}$), field capacity ($0.38 \text{ cm}^3 \text{ cm}^{-3}$) and saturation ($0.46 \text{ cm}^3 \text{ cm}^{-3}$).

2.2.3 Crop growth and phenology

For model calibration, total above dry matter and leaf area index at 20 day after emergence, at beginning of flowering, beginning of pod formation, beginning seed formation, full seed and after full maturity were measured in Piracicaba and Frederico Westphalen.

Harvest yield at maturity, harvest index, planting date, emergence, anthesis, beginning of pod formation, beginning of seed formation and maturity days were also measured in Piracicaba, Londrina and Frederico Westphalen. For the evaluation process, yield at maturity and dates of each crop phase were measured in Piracicaba and Frederico Westphalen; while for test of cultivars only sowing date and yield at maturity were obtained. More details about crop growth and phenology evaluation are presented in Appendix C.

2.2.4 Crop models

Soybean growth and development were simulated by five crop models, as follows: FAO – Agroecological Zone (KASSAM, 1977; DOORENBOS; KASSAM, 1979; RAO et al., 1988), referred as FAO; FAO – AQUACROP v. 4.0 (STEDUTO et al., 2009; RAES et al., 2012), referred as AQUACROP; Model for Nitrogen and Carbon in Agroecosystems v. 2.11 (NENDEL et al., 2011), referred as MONICA; Crop System Model – CROPGRO – Soybean v. 4.6.1 presented in the software Decision Support System for Agrotechnology Transfer (BOOTE et al., 1998, 2003; JONES et al., 2003), referred as DSSAT; and Agricultural Production Systems Simulator v. 7.7 (ROBERTSON; CARBERRY, 1998; KEATING et al., 2003; HOLZWORTH et al., 2014), referred as APSIM. In Annex C and Appendix D are describe more details about the crop models.

2.2.5 Calibration phases

The crop models were calibrated in three phases, always comparing the estimated with measured data. In the first phase, the aim was to evaluate the efficiency of simulations without any calibration by using observed weather, soil profile and management (sowing date, irrigation, fertilization and initial condition) for the locations previously mentioned, adopting a calibrated cultivar with cycle similar to BRS 284, available in the models. In the second phase, only the coefficients associated to crop phenology were calibrated, including the following crop stages: emergence; beginning of flowering; beginning of pod; beginning of seed formation; and maturity. The third phase considered also the calibration of crop growth coefficients (above and below the soil). The best calibration was considered when the lowest differences between predicted and measured yield, total dry matter, leaf area index and harvest index were obtained.

2.2.6 Data analysis

The models performance was obtained comparing the values of yield, harvest index, leaf area index, total above-ground biomass and crop phases predicted by each model and mean from models ensemble against measured values in the 2013/14 crop season. For the 2014/15 crop season, these data were used to model evaluation covering soybean grain yield. For DSSAT, APSIM and MONICA were compared all variables, while for AQUACROP was not included leaf area index, and for FAO was compared only yield. Root mass, evapotranspiration and available water in the soil simulated were analysis to compare the values predicted between crop models. The root mass was not analyzed for FAO model, due to the model not simulate this variable.

The results obtained by the crop models and their ensemble were compared to measured field experimental data after each calibration phase and the following statistical indices and errors were used for their evaluation (WALLACH et al., 2006): bias; mean absolute error (MAE); Willmott agreement index (D) (WILLMOTT et al., 1985); root mean square error (RMSE); coefficient of determination (r^2). Graphics with the relationship between measured and estimated yields were also used, as well as graphics of residual error versus measured yield.

2.3 Results and Discussion

2.3.1 Crop model performance

Soybean grain yield

Most of crop models showed an improvement of performance from phase one, without calibration, to phase three, with complete calibration (Table 2), except the FAO model that had its performance reduced from phase 2 to 3, due to the use of observed harvest index. In this case, an average value of HI proposed by Battisti (2013), used in phase 2, was more efficient for yield estimation. Although improvement of performance was observed for phase 3, FAO and APSIM crop models showed a good performance even in phase one and two, with RMSE lower than 769 kg ha^{-1} and d index higher than 0.85. On the other hand, AQUACROP showed a poor estimation of soybean yield in these two first phases, with a negative bias of about 1700 kg ha^{-1} , which was highly improved in the phase three, when

growth coefficients were calibrated. APSIM, DSSAT and MONICA showed a respective yield RMSE of 653, 759 and 1063 kg ha⁻¹ in phase two, showing that growth coefficients from models' default are close to those used for the Brazilian cultivar BRS 284.

The coefficients used in the FAO model in phase one were obtained in a study developed in the same region of field experiments. For APSIM, DSSAT and MONICA, these coefficients were from a cultivar of the same maturity group of BRS 284, whereas for AQUACROP, the coefficients were from an unknown cultivar, but probably from a higher maturity group, with longer cycle and lower growth rate. Jégo et al. (2010) verified similar condition using the STICS crop model for wheat and soybean in Canada, where the model needed less calibration in wheat than soybean cultivars, due to coefficient for wheat cultivars in STICS represent better the cultivars used in the region than soybean.

Table 2 – Crop model performance for soybean grain yield in the three phases of calibration

Crop Model	Phase ¹	Bias	MAE	RMSE	d	r ²	Predicted ²	Measured ²
		Kg ha ⁻¹					Kg ha ⁻¹	
FAO	P1	136	445	563	0.88	0.66	3019	
	P2	22	332	440	0.92	0.79	2905	
	P3	124	526	650	0.91	0.79	3006	
AQUACROP	P1	-1718	1824	2010	0.37	0.00	1164	
	P2	-1769	1769	1958	0.42	0.39	1113	
	P3	165	458	536	0.91	0.71	3047	
DSSAT	P1	957	1061	1397	0.72	0.60	3839	
	P2	175	615	759	0.87	0.66	3058	
	P3	65	444	548	0.93	0.79	2948	2883
APSIM	P1	579	664	769	0.85	0.75	3462	
	P2	180	530	653	0.86	0.57	3062	
	P3	156	440	550	0.90	0.69	3038	
MONICA	P1	1381	1409	1622	0.61	0.49	4264	
	P2	833	883	1063	0.74	0.58	3716	
	P3	-26	429	535	0.92	0.72	2856	
Ensemble of models ³	P1	267	398	518	0.91	0.77	3150	
	P2	-112	385	464	0.92	0.78	2771	
	P3	97	218	262	0.98	0.93	2979	

¹P1 is phase 1, without calibration, P2 is phase 2, calibrating only crop development, P3 is phase 2, with complete calibration; ²Predicted and measured is the average of seventeen results; ³Index estimating using the average of yield from all models

The models showed a similar performance in phase three for bias, between -26 (MONICA) and 165 kg ha⁻¹ (AQUACROP), index d, between 0.90 (APSIM) and 0.93 (DSSAT), and r², between 0.69 (APSIM) and 0.79 (FAO) (Table 12). For MAE and RMSE,

the values were similar among all models, except for FAO, which had higher MAE (526 kg ha⁻¹) and RMSE (650 kg ha⁻¹) (Table 2). These results are similar or even better than those obtained in other studies. For DSSAT, Boote et al. (2003) and Bao et al. (2015) obtained, respectively, a RMSE between 226 and 650 and 201 and 413 kg ha⁻¹, while for APSIM, Mohanty et al. (2012) obtained a bias of 100 kg ha⁻¹ for soybean. Paredes et al. (2015) obtained with AQUACROP in China a bias ranging from -499 to 415 kg ha⁻¹ for soybean, and Battisti and Sentelhas et al. (2015) obtained bias of 7 kg ha⁻¹, MAE of 284 kg ha⁻¹ and index d of 0.87 for FAO model in Brazil. For MONICA no results for soybean were found in the literature.

The soybean grain yield estimates were improved when ensemble of models was employed. Ensemble of models resulted in a better statistical performance than any of the soybean models used individually, with MAE = 218 kg ha⁻¹ and RMSE = 262 kg ha⁻¹ (Table 2), which represent half of the errors obtained previously with any single model after completely calibrated. The ensemble of models has been used in the past largely for simulations of climate conditions, and presently, ensemble has been tested and used for yield estimation by crop models, in an approach known as multi-model (VANUYTRECHT et al., 2011). According to Martre et al. (2015), ensemble of models is better than used only a single model, since different crop models vary with their nature in terms of processes simulated, environmental conditions and objectives of the study for which they were developed (ASSENG et al., 2013)

The crop models also need to be able to simulate yields in different environmental conditions, from dry (JAMIESON et al., 1998) to wet (PORTER et al., 1993). Figure 2 shows the relationship between soybean grain yields observed in the field experiments and simulated by the crop models. In the experiments yield ranges from 1000 to 5000 kg ha⁻¹, showing the huge environmental variability faced by the soybean crops. Most of models showed a slight tendency of overestimating yields, between 2.8% for APSIM (Figure 2d) and 6.2% for FAO (Figure 2a). The only exception was for MONICA model which underestimated yields by 1.6% (Figure 2e). The ensemble of models had clearly better performance than any single model, with the lowest data dispersion ($r^2 = 0.93$) and an overestimation of 2.7% (Figure 2f). The major differences captured by the models can be attributed to differences in crop management, the second most importance source of yield gap for soybean in Brazil (SENTELHAS et al., 2015). Despite these differences, the models and their ensemble were able to estimate yield variability, which means that they can simulate the impact of environmental conditions on yield, as observed for by Pirttioja et al. (2015).

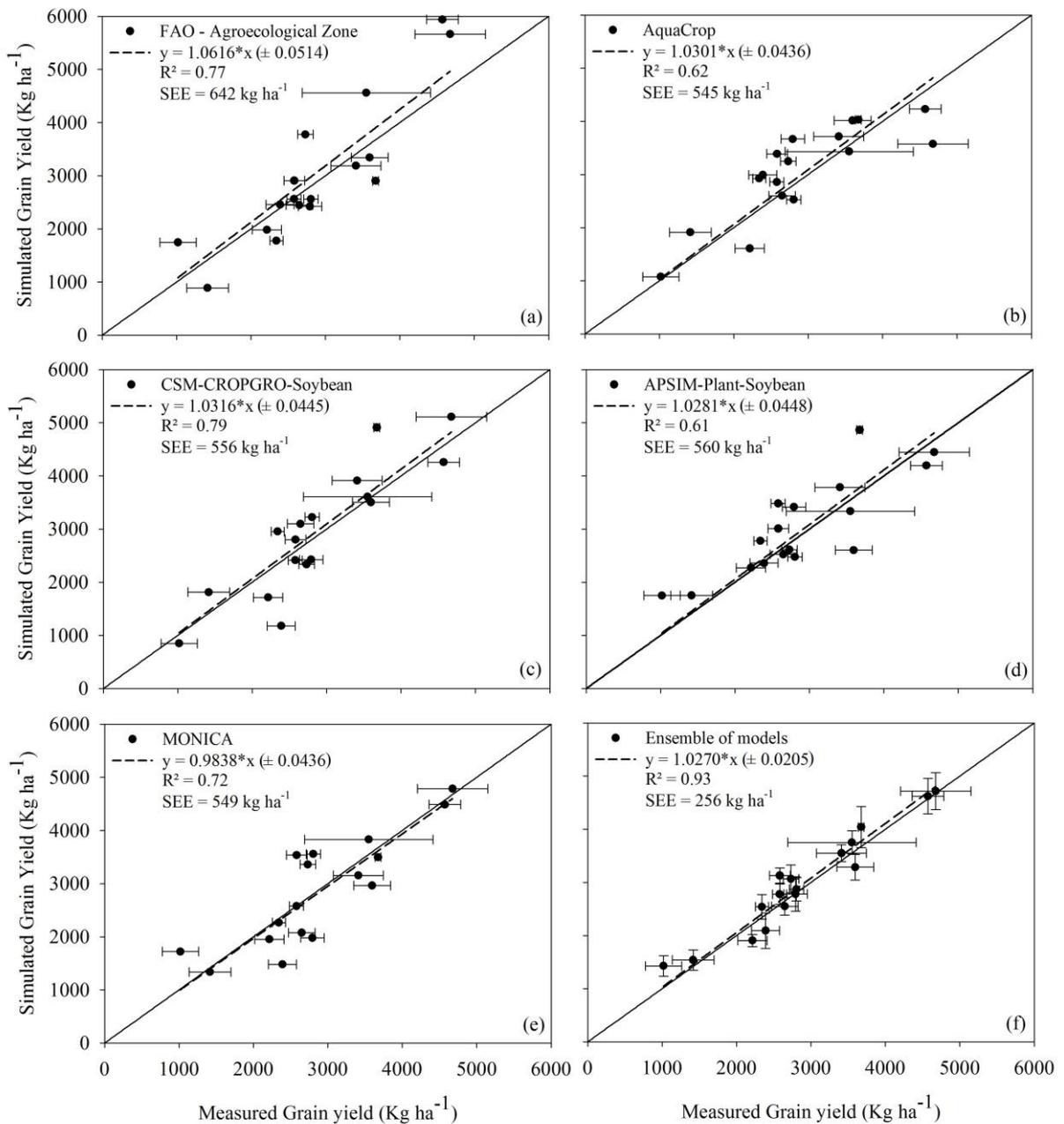


Figure 2 – Relationship between measured and simulated soybean grain yield using five full calibrated crop simulation models for soybean: FAO (a); AQUACROP (b); DSSAT (c); APSIM (d); MONICA (e); and models' ensemble (f). The bars indicate standard deviation for estimated and observed values and \pm is standard error for equation

The models' ensemble resulted in a reduction of errors when compare with the results from the single models, showing error between -500 and 500 kg ha^{-1} (Figure 3), which represent less than 17%. As single models, the ensemble also showed a higher relative error (40%) for the lower yields, showing that there is some limitation in these models to simulate yield under extreme water deficit. For the other yield levels, the relative errors caused by the

ensemble were below 20%. Martre et al. (2015) also observed a better performance of yield simulations when the ensemble of the 27 wheat models was used in different regions in the world, with RMSE varying between 410 and 490 kg ha⁻¹, respectively for median and mean grain yields, against 420, 560 and 630 kg ha⁻¹ for the first, second and third best single models.

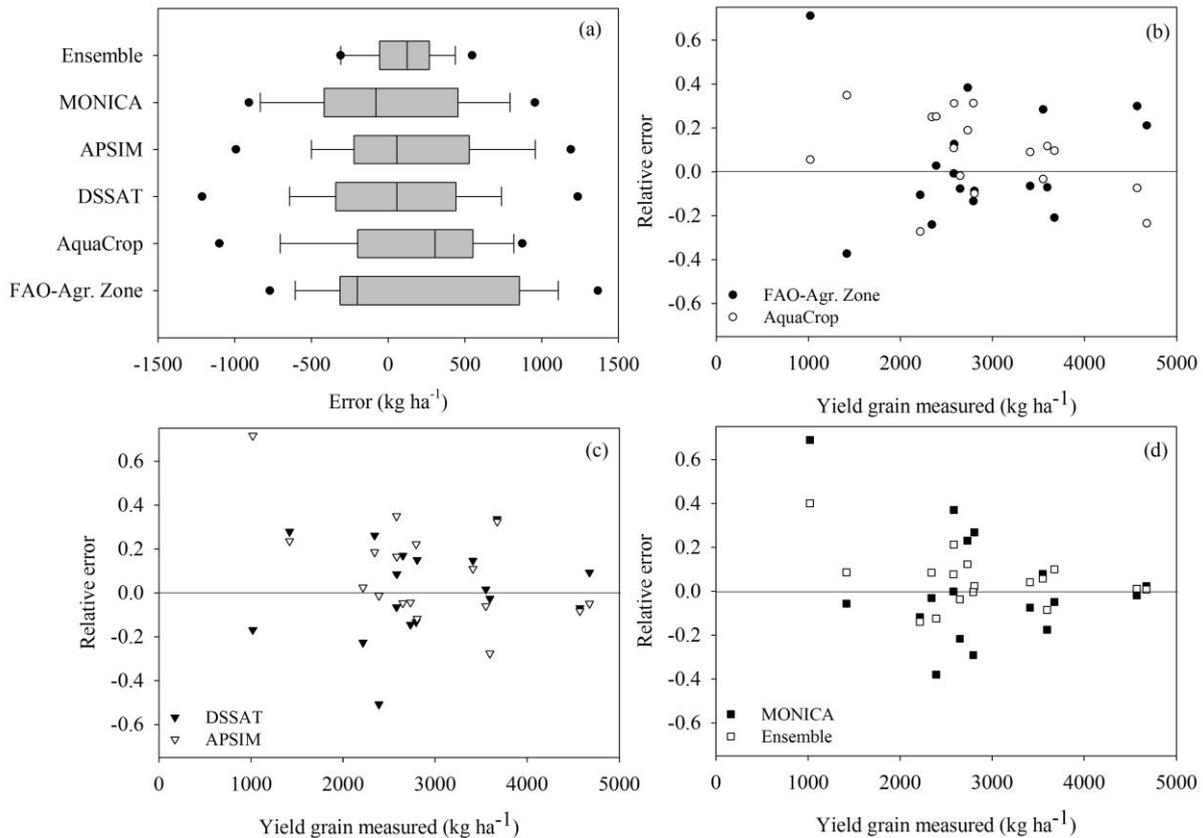


Figure 3 – Error distribution for yield simulated for five crop models and from ensemble of models (a), and relative error in function of observed yield for FAO-Agroecological zone and AquaCrop (b), DSSAT and APSIM (c), and MONICA and using ensemble of these models (d)

The overestimation of yield under extreme water deficit observed in this study highlights an important aspect that needs to be improved in the crop models, which are related to root growth and soil extractable water. In DSSAT, for example, rooting is adjusted using a coefficient of root distribution in the soil profile (MA et al., 2009), information that can be found more easily for the study region than the parameters of maximum water uptake for each day per soil layer, which is used by APSIM (DARDANELLI et al., 1997). These variables related to soil and roots require a local calibration due to the interaction of crop and soil characteristics. In this context, Palosuo et al. (2011) discussed other interesting aspects such

as the definition of maximum root depth in the models, which can be considered as the maximum depth with roots presence or the maximum depth with the effective root system. These definitions change the soil water availability for the crop and therefore the simulated yields, mainly under water deficit.

Crop phases

The crop phase dates were well estimated by different crop models, especially for beginning of flowering (R1) and maturity (R7) (Figure 4a), once these phases are better defined in all models than beginning of pod formation (R3) and beginning of grain filling (R5). The RMSEs were reduced from phase 1 of calibration to phase 3, when R1 date presented a RMSE lower than 4 days (Figure 4b). No results are presented for AQUACROP since the original coefficients in the model are for a cultivar with longer cycle, which makes it impossible to simulate R1 and R7 dates. Although the AQUACROP model considers only thermal time to estimate R1 date (RAES et al., 2012), the performance of this model when calibrated was very close to MONICA, APSIM and DSSAT models, which consider the interaction of thermal time and photoperiod sensitivity (Figure 4). For R7, the RMSE was also reduced going from phase 1 (< 12 days) to phase 3 (< 7 days) for MONICA model, whereas the better performance was obtained by DSSAT and APSIM, with RMSE lower than 5 days (Figure 4b). The FAO model was not included in this analysis, since this model uses fixed crop phases.

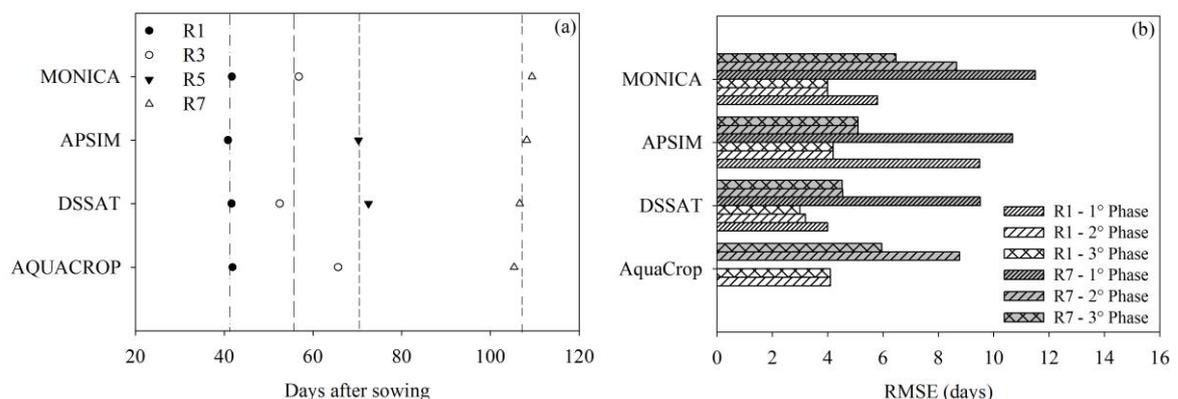


Figure 4 – Days after sowing for flowering (R1), beginning of pod formation (R3), beginning of grain filling (R5) and maturity (R7) observed (lines) and simulated (points) by different crop models (a) and root mean square error for date of occurrence of R1 and R7 in three phases of calibration (b)

DSSAT and APSIM were the best crop simulation models to estimate crop phenology. The main reason for that, besides the use of thermal time and photoperiod sensitivity coefficients, is the influence of water deficit and nitrogen limitation on crop development rate (SPECHT et al., 2001). In this way, Ruíz-Nogueira et al. (2001) observed that the adjustment of water-stress induced acceleration of maturity for water deficit conditions in DSSAT contributed for reducing biomass and grain yield errors.

The dates R3 and R5 were measured based on Fehr and Caviness (1977) phenology scale, which has different definitions when compared with the crop models. For the crop models R3 is the occurrence of first pod and R5 is the occurrence of first seed (R5). This mismatch led to higher errors for R3 and R5 than for R1 and R7 (Figure 4a). Palosuo et al. (2011) also observed similar problem for wheat models. The wrong crop phase estimation can lead also to yield errors, once yield formation phase is of major importance to define harvest index. Therefore, the grain filling phase requires to be properly calibrated for accurate yield estimation, by considering model structure, yield formation phase, cultivar growth habit and dry mass partitioning. Martre et al. (2015) mentioned that the solution of these inconsistencies in crop phases R3 and R5, can help to improve soybean crop models' performance.

Total above-ground biomass, harvest index and leaf area index

The crop models showed an improvement of performance to estimate total above-ground biomass (TAGB) from phase one to phase three of calibration (Table 3). The AQUACROP, DSSAT and APSIM had underestimation in phase three with an estimate, respectively, of 5504, 5149 and 5205 kg ha⁻¹ against 6090 kg ha⁻¹ observed at field, considering the average of six evaluation along crop cycle. On the other hand, full calibrated MONICA overestimated TAGB by 421 kg ha⁻¹, while the ensemble of models had a bias of -498 kg ha⁻¹. Full calibrated models showed a good agreement between estimated and observed values, presenting $d > 0.88$ and $r^2 > 0.80$. It is important consider growth variables in crop model evaluation because good prediction of crop yield can be due to a wrong reason, if the models overestimating or underestimating total biomass or harvest index, for example (PALOSUO et al., 2011; MARTRE et al., 2015).

TAGB estimated by the crop models resulted in RMSEs between 2284 (37%) and 2700 (44%) kg ha⁻¹ (Table 3), which according to Jégo et al. (2010) can be consider an unsuitable performance, meaning that improvements in the models/calibrations are required. Despite these errors, the models were able to simulate the crop growth curve appropriately,

for both rainfed and irrigated conditions, with similar values between observed and simulated at harvest (last point at Figure 5). The accurate model calibration for crop growth variables is an important aspect in crop modeling because wrong calibrations can lead to a compensation process, which may result in a good yield prediction but based on wrong assumptions. Such fact can result in estimated yield inconsistencies under different soil/climate conditions (PALOSUO et al., 2011; MARTRE et al., 2015).

Table 3 – Crop model performance for six time series samples for soybean total above-ground biomass (TAGB) in the three phases of calibration

Crop Model	Phase ¹	Bias	MAE	RMSE	d	r ²	Predicted ²	Measured ²
		Kg ha ⁻¹					Kg ha ⁻¹	
AQUACROP	P1	-1593	2267	3394	0.84	0.64	4497	
	P2	-3980	4052	5659	0.57	0.66	2110	
	P3	-587	1758	2700	0.88	0.80	5504	
DSSAT	P1	-878	1439	2392	0.92	0.81	5212	
	P2	-1227	1486	2535	0.91	0.85	4863	
	P3	-941	1322	2284	0.93	0.87	5149	
APSIM	P1	-448	1438	2189	0.94	0.83	5642	
	P2	-667	1405	2252	0.93	0.85	5424	6090
	P3	-886	1490	2403	0.92	0.85	5205	
MONICA	P1	516	2033	2699	0.89	0.73	6606	
	P2	757	2096	2653	0.90	0.75	6848	
	P3	421	1756	2364	0.92	0.82	6511	
Ensemble ³	P1	-601	1481	2409	0.92	0.81	5489	
	P2	-1279	1669	2884	0.86	0.83	4811	
	P3	-498	1396	2306	0.92	0.92	5592	

¹P1 is phase 1, without calibration, P2 is phase 2, calibrating only crop development, P3 is phase 2, with complete calibration; ²Predicted and measured is the average of seventeen experiment sampled six times over cycle; ³Index estimating using the average of total above-ground biomass from all models

As observed for TAGB, all models had their performance for estimating harvest index improved when fully calibrated. For AQUACROP, RMSE was reduced from 0.273 (72%) to 0.081 (21%), respectively from calibration phase 1 to 3, whereas APSIM model showed similar results between estimated (0.36 – 0.38) and measured (0.38) harvest index (Table 4). For the ensemble of models, the performance was better, with bias = -0.017, RMSE = 0.065 and d = 0.63. Kahlon et al. (2011) reported that old soybean cultivars had smaller number of seeds and pods per square meter than new ones with higher yield potential. A well-defined harvest index is required for accurate yield estimation, especially if model's default values are from cultivars that are not being used by growers anymore.

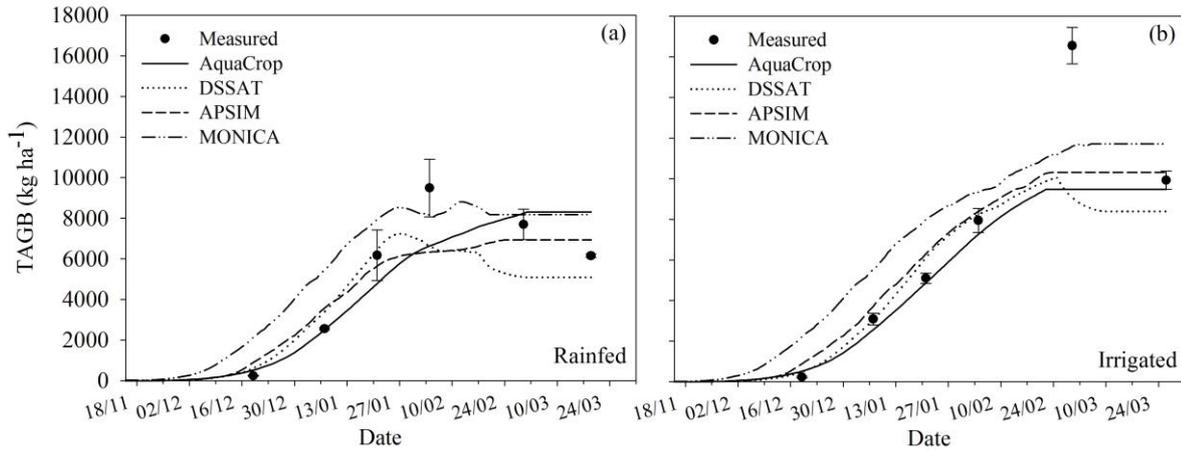


Figure 5 – Soybean total above-ground biomass (TAGB) measured and predicted by four crop models fully calibrated under rainfed (a) and irrigated (b) conditions, in Piracicaba, SP, Brazil, with sowing date on 14/Nov/ 2013. The bars indicate standard deviation of measured values

Table 4 – Crop model performance for soybean harvest index in the three phases of calibration

Crop Model	Phase ¹	Bias	MAE	RMSE	d	R ²	Predicted ²	Measured ²
		Kg kg ⁻¹					Kg kg ⁻¹	
AQUACROP	P1	-0.253	0.253	0.273	0.26	0.14	0.13	
	P2	-0.056	0.077	0.097	0.41	0.02	0.33	
	P3	-0.027	0.066	0.081	0.39	0.01	0.35	
DSSAT	P1	0.142	0.144	0.157	0.48	0.29	0.52	
	P2	0.090	0.106	0.122	0.53	0.16	0.47	
	P3	0.056	0.080	0.094	0.64	0.26	0.44	
APSIM	P1	-0.002	0.048	0.058	0.68	0.32	0.38	
	P2	-0.019	0.054	0.071	0.44	0.06	0.36	0.38
	P3	-0.005	0.048	0.061	0.65	0.25	0.38	
MONICA	P1	0.006	0.083	0.108	0.33	0.04	0.39	
	P2	-0.046	0.073	0.104	0.36	0.01	0.34	
	P3	-0.094	0.097	0.121	0.49	0.13	0.29	
Ensemble ³	P1	-0.027	0.056	0.076	0.43	0.04	0.35	
	P2	-0.008	0.052	0.070	0.47	0.06	0.37	
	P3	-0.017	0.048	0.065	0.63	0.23	0.36	

¹P1 is phase 1, without calibration, P2 is phase 2, calibrating only crop development, P3 is phase 2, with complete calibration; ²Predicted and measured is the average of seventeen results; ³Index estimating using the average of harvest index from all models

Harvest index is a parameter associated to physiologically-based processes in the models (JAMIESON et al., 1998), with this index being dependent on dry matter partitioned to the grain during grain filling period and environmental conditions of different sites, sowing dates and cultivars (BOOTE et al., 2003; LAWN; JAMES, 2011). Figure 6 presents the relationship between measured and simulated harvest indices for DSSAT and AQUACROP.

In this analysis, DSSAT, a more complex model, had a clear correlation between these values, with bias = 0.056, RMSE = 0.094 and $d = 0.64$, despite the overestimation observed, whereas AQUACROP, a simpler model, presented a poor correlation, with simulated values almost not varying. The overestimation can be caused by presence of leaf and petiole mass at harvest, while in the crop model, these are considered drop to compute harvest index.

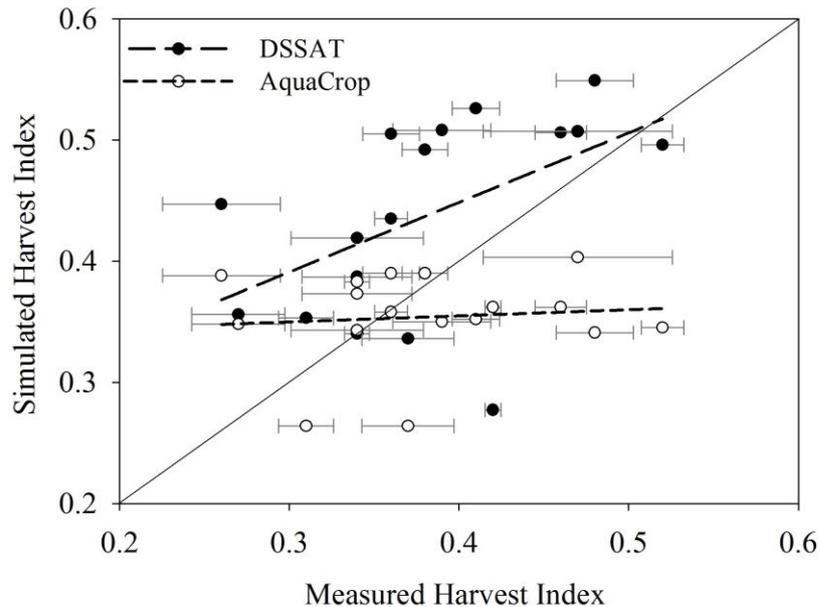


Figure 6 – Relationship between measured and simulated harvest index by DSSAT and AQUACROP model. The bars indicate standard error of measured values

Leaf area index (LAI) analysis was not included with the FAO and AQUACROP models, since they do not estimate this variable. FAO simply considers a fixed value for each crop phases, whereas AQUACROP uses canopy cover index (RAES et al., 2012). For DSSAT and APSIM models, the LAI presented lower bias, MAE and RMSE than MONICA model, which had a bias = 1.18 in phase 3 of calibration (Table 5). For all calibration phases, the comparison between measured and estimated LAI resulted in $d > 0.82$ and $r^2 > 0.60$. The models' ensemble, when applied, reduced RMSE by 6%, estimating LAI better than any single crop model.

The crop models were also able to simulate the LAI for rainfed and irrigated crops, as observed in Figure 7. Under rainfed conditions, the models simulated reduction of leaf area index from the middle to the end of crop cycle, due to water deficit (Figure 7a), with a more drastic LAI decline for APSIM and DSSAT, and less drastic for MONICA. Under irrigated conditions (Figure 7b), DSSAT and APSIM models sustained LAI until maturity (5th LAI assessment), after when the models simulated senescence.

Table 5 – Crop model performance for leaf area index for soybean in the three phases of calibration

Crop Model	Phase ¹	Bias	MAE	RMSE	d	r ²	Predicted ²	Measured ²
		m ² m ⁻²					m ² m ⁻²	
DSSAT	P1	-0.11	1.07	1.48	0.85	0.60	2.50	
	P2	0.03	0.86	1.25	0.91	0.71	2.65	
	P3	0.01	0.83	1.22	0.92	0.73	2.62	
APSIM	P1	0.16	0.84	1.16	0.93	0.76	2.78	
	P2	-0.20	0.90	1.35	0.90	0.67	2.42	
	P3	-0.32	0.94	1.40	0.89	0.66	2.29	2.62
MONICA	P1	1.47	1.60	2.13	0.82	0.65	4.08	
	P2	1.35	1.48	1.95	0.84	0.69	3.97	
	P3	1.18	1.34	1.73	0.88	0.75	3.79	
Ensemble	P1	0.51	0.95	1.27	0.91	0.75	3.12	
	P2	0.40	0.87	1.22	0.92	0.75	3.01	
	P3	0.29	0.82	1.15	0.93	0.77	2.90	

¹P1 is phase 1, without calibration, P2 is phase 2, calibrating only crop development, P3 is phase 2, with complete calibration; ²Predicted and measured is the average of seventeen experiment sampled six times over cycle; ³Index estimating using the average of leaf area index from all models

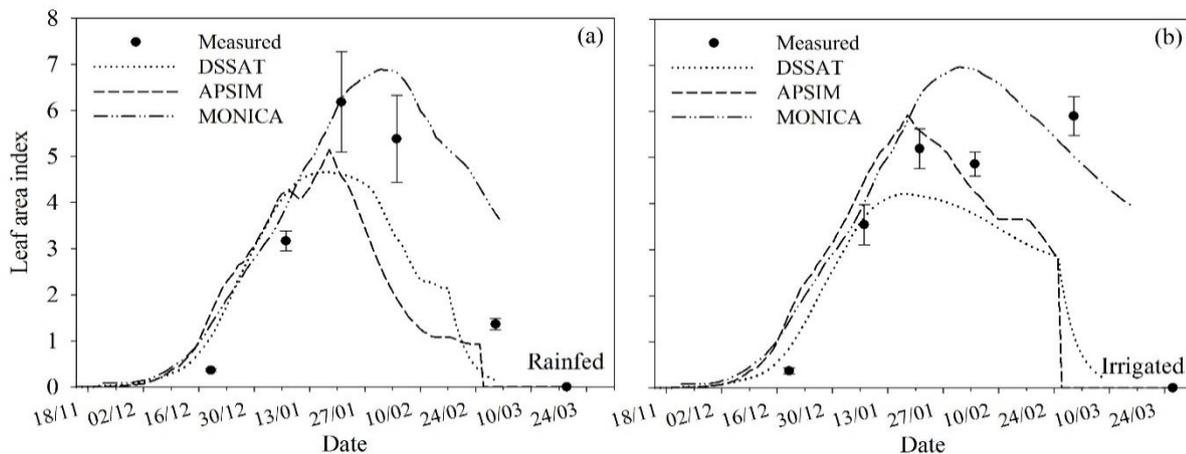


Figure 7 – Leaf area index measured and predicted by four crop models under rainfed (a) and irrigated (b) conditions in Piracicaba for sowing date in Nov 14th, 2013. The bars indicate standard error of measured values

Evapotranspiration, water content on the soil and root density and mass

Evapotranspiration, water content on the soil and root density and mass are important variables considered in the crop models and affect directly soybean yield, especially in Brazil, where water deficit is the main concern and yield gap (SENTELHAS et al., 2015). Although these variables were not measured at field experiment, it is made an analysis of different values simulated by the crop models for a specific field experiment sowing in Nov 14th at Piracicaba under rainfed and irrigated conditions.

The potential and actual evapotranspiration simulated by five crop models had APSIM with higher value, reaching 12 mm day^{-1} , model that use transpiration efficiency approach (AGRICULTURAL PRODUCTION SYSTEMS SIMULATOR - APSIM, 2015), being follow by FAO with 10 mm day^{-1} , while DSSAT, MONICA and AQUACROP had maximum value around of 8 mm day^{-1} (Figure 8). Sau et al. (2004) also verified difference on evapotranspiration using different equations to the potential evapotranspiration and to partition in evaporation and transpiration in the DSSAT-CROPGRO-Fababean model. In the field experiment, Berlato et al. (1986) observed evapotranspiration values between 6 and 7.5 mm day^{-1} during maximum demand of soybean, where the difference between this study and the models can be associated with climate conditions in the field experiment.

The approaches used by crop models to estimate evapotranspiration creating different curve to evapotranspiration over crop cycle (Figure 8). The model MONICA and FAO use a approach based in a potential value multiply by crop coefficient (K_c) to estimate evapotranspiration, and because this, the curve begin lower and increase until 80 days after sowing and after reduce until maturity. The other models, DSSAT, APSIM and AQUACROP, do not follow curve pattern of crop coefficient, because there is a balance between evaporation and transpiration, being evaporation higher in the beginning of cycle and decreasing with increase of leaf area, moment that transpiration increase due to higher solar radiation interception.

The models had similar moment where water deficit is simulated, which can be observed by the difference between potential and actual evapotranspiration (Figure 8). The water deficit occurred at the beginning of cycle, between 20 and 40 days after sowing, for all models, except to MONICA, due to higher root growth and lower evapotranspiration demand. Other moment that models simulate water deficit was from the middle to the end of cycle, being between 60 to 100 days after sowing, during grain filling of soybean. The results showed that the models are agreeing for limitation by water that penalizes soybean yield.

In the models, different values were used to maximum depth root based in the approach used to water uptake. As showed in Figure 9, the DSSAT and APSIM had highest water available in the soil, higher than 250 mm in the beginning of cycle, due to these models consider a maximum root depth of 150 cm. The model MONICA had the value around of 100 mm, but for a root depth of 75 cm, value defined during calibration. For AQUACROP, it was defined during calibration a maximum root depth of 110 cm, resulting in maximum water available of 150 mm (Figure 9d). For FAO (Figure 9e), there is two maximum depth, of 60 cm to rainfed condition, and 50 cm to irrigated, because we assume that under rainfed

conditions the roots increased on depth (HOSSAIN et al., 2014), where water available reach maximum values close of 100 mm.

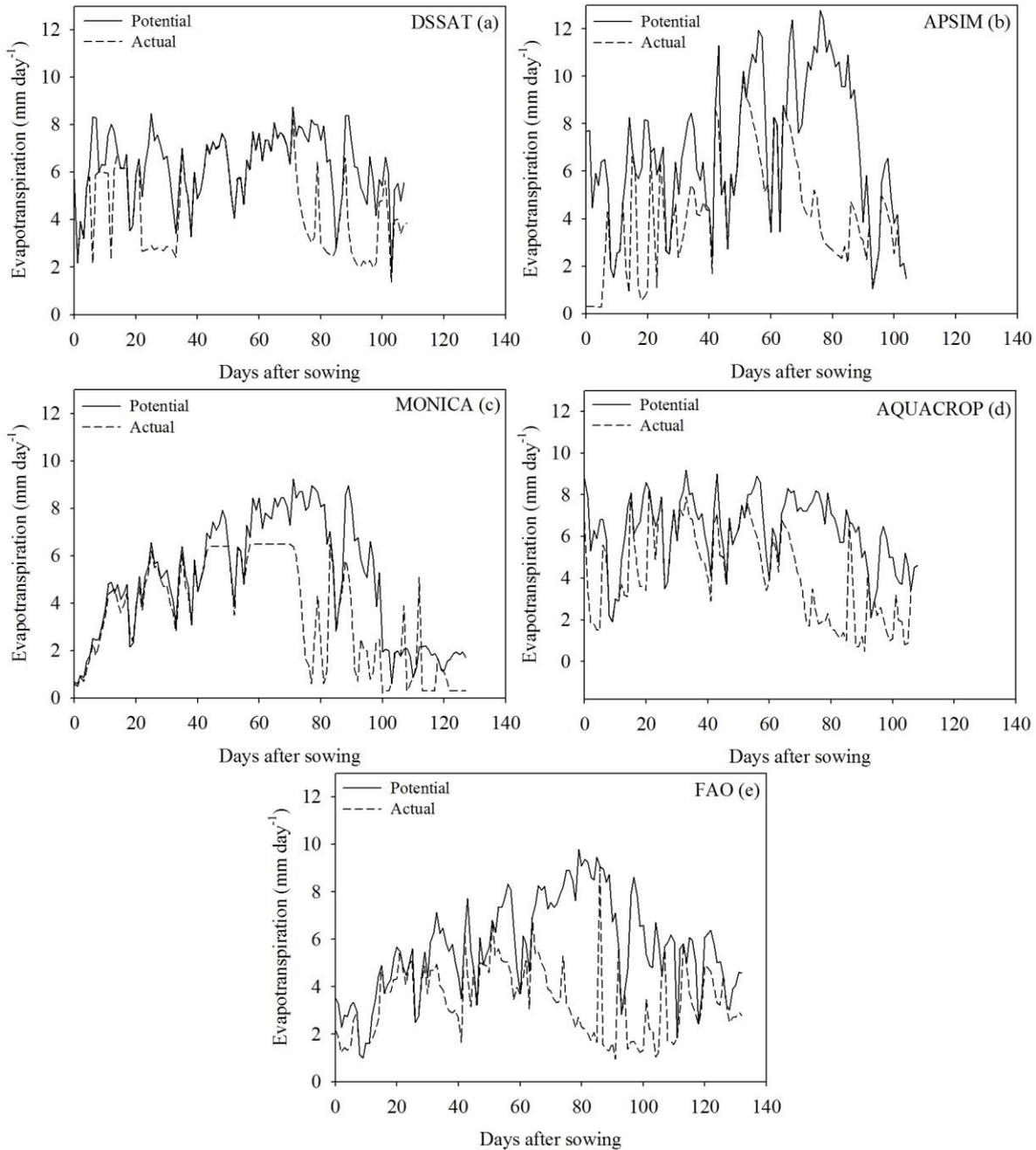


Figure 8 – Potential and actual crop evapotranspiration estimated by five crop models, DSSAT (a), APSIM (b), MONICA (c), AQUACROP (d) and FAO (e), after calibration for the field experiment sowing in Nov 14th under rainfed condition at Piracicaba, SP

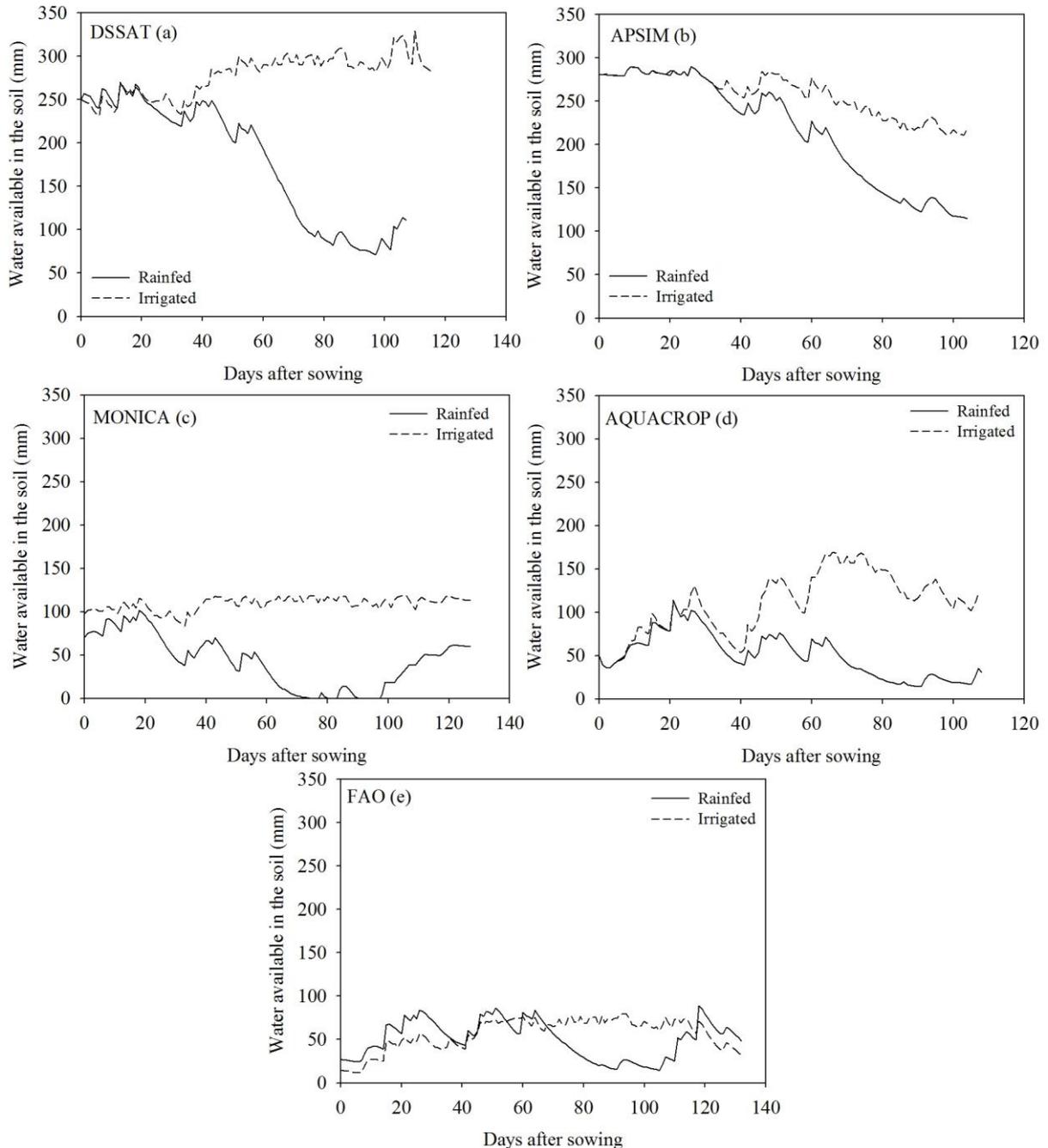


Figure 9 – Water available in the soil to the crop estimated by five crop models, DSSAT (a), APSIM (b), MONICA (c), AQUACROP (d) and FAO (e), after calibration for the field experiment sowing in Nov 14th under rainfed and full irrigated condition at Piracicaba, SP. Water available is the difference between water content and permanent wilting point after drainage

DSSAT, APSIM and MONICA had a constant value of water available in the soil to the crop because the output from the model consider all soil profile, while AQUACROP and FAO had the output based in the current root depth. In this context, the values of water available, shown in Figure 9 not means that all water is available to water uptake, because DSSAT, APSIM and MONICA consider water uptake a function of root density in each soil

layer, while AQUACROP and FAO use an index to limit water uptake due to reduction of water in the soil.

DSSAT and APSIM are models that simulate root density along soil profile. The most root density was simulate in the upper of soil, being reduce in depth (Figure 10a). The soil root exploration is also dependent of root mass, condition that is dependent of total biomass produce by the crop and fraction that is diverge to root. The models also consider effect of water deficit to diverge dry mass to root growth, where in Figure 10b is shown the difference between rainfed and irrigated condition for APSIM, DSSAT and MONICA.

APSIM, DSSAT and MONICA also had different curve to root mass along crop cycle (Figure 10b). DSSAT consider the reduction of root mass due to senescence, while APSIM and MONICA not did. Other point was rate of growth, where DSSAT and APSIM had a similar rate of growth, while MONICA had a higher rate root growth than other models (Figure 10b). This higher rate of root growth to MONICA can be the cause to the model not showed water deficit in the beginning of cycle, as showed previous in Figure 8c.

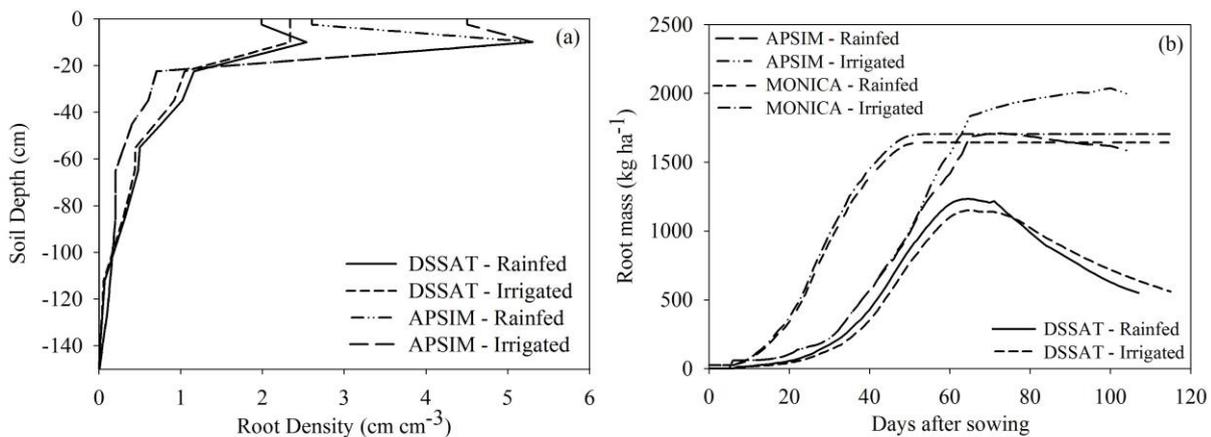


Figure 10 – Root density at 70 days after sowing estimated by DSSAT and APSIM (a) and root mass along crop cycle estimated by DSSAT, APSIM and MONICA (b) after calibration for the field experiment sowing in Nov 14th under rainfed and irrigated condition at Piracicaba, SP

2.3.2 Performance of the calibrated models with independent data

The yield data that were not used in the calibration process of the models were applied to test them. This analysis resulted in huge data dispersion, with RMSE always above 1000 kg ha⁻¹ when considered single models and RMSE = 981 kg ha⁻¹ when considering the ensemble (Figure 11). These results can lead to a wrong conclusion about model performance. In this

analysis, it is important to realize that there are limiting aspects for each one of the models, mainly associated to weeds, pests and diseases (RODRIGUES et al., 2013), and also to the inputs for the models (PALOSUO et al., 2011; KERSEBAUM et al., 2015).

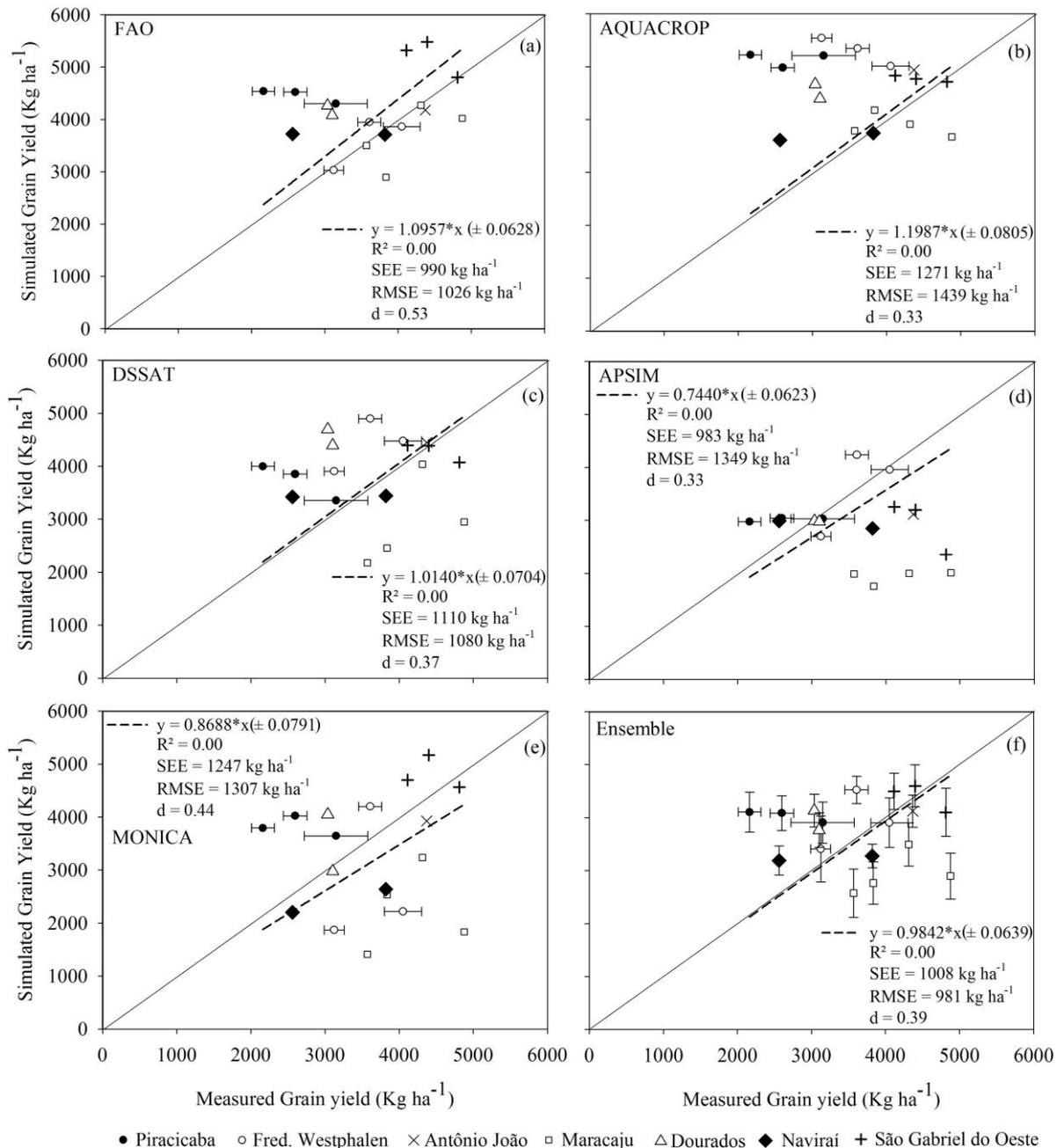


Figure 11 – Relationship between measured and simulated soybean grain yield using five full calibrated crop simulation models for soybean: FAO (a); AQUACROP (b); DSSAT (c); APSIM (d); MONICA (e); and models' ensemble (f), using independent date. The bars indicate standard error and \pm is standard error for equation

Analyzing the results for Piracicaba (three sowing dates in 2014/2015 crop season) is possible to observe that all models overestimated soybean grain yields (Figure 11). In this field experiment a high Asian rust pressure was observed that resulted in severe yield loss. Another source of error is when the soil and climatic data are not exactly close to the experimental site, when analyzing the data from the cultivar test trial. So, even using representative soil data of each soil type and weather data from the closest station, this information can lead to errors; however of low magnitude.

2.3.3 Coefficients calibrated

The mainly coefficients calibrated for the five crop model are showed in Table 6. These values were obtained in phase 3 of calibration, where coefficients related with crop development and growth were adjusted. Parameters related with soil, such as soil root growth factor (SRGF) in DSSAT and limit fraction of water available to be extracted per day in each layer (KL) in APSIM, also were adjusted to improve crop model performance, altering root growth and root water uptake, affecting the level of water deficit simulated by crop models. The all coefficients description and values for phase 1, 2 and 3 for all models and the four values for APSIM crop development are showed in Annex D, E, F, G, H to I. The crop models have different number of coefficients and although the traits have the same definition, the values of coefficients are different due to crop model architecture. The number of coefficients and the transparency of crop models are an important point to be considered.

2.3.4 Overall performance

The crop models are chosen since that appropriate for the objective, robustness to predicted efficiently the crop results in the region and transparency, with parameters, flow diagrams and code accessible (SOLTANI; SINCLAIR, 2015), points used here to analysis overall performance of models. Other important points is the user knowledge how to calibrate, use the model and the limiting points that need to be observed. As comments by Soltani and Sinclair (2015), if the developer calibrate the crop model, the performance probably will be better than if the calibration was did by a simple user, due to the developer know the structure and limiting points.

Table 6 – Summary of coefficients calibrated for each soybean crop model in the three phase of calibration processes

(continued)			
Trait ¹	Value	Trait	Value
FAO		FAO	
Ky S-V2	0.05	Ky V2-R1	0.15
Ky R1-R5	0.4	Ky R5-R7	0.75
Ky R7-R8	0.1	MRD Irrigated	50
MRD Rainfed	60		
DSSAT		DSSAT	
CSDL	13	PPSEN	0.369
EM-FL	24.7	FL-SH	6.5
FL-SD	18.5	SD-PM	30
FL-LF	26	LFMAX	1.12
SLAVR	340	SIZELF	185
XFRT	1	WTPSD	0.21
SFDUR	23	SDPDV	2.3
PODUR	12	THRSH	74
SDPRO	0.4	SDLIP	0.2
FL-VS	26	RHGHT	1
SRGF ² Layer 1 (0 - 5 cm)	1.00	SRGF ² Layer 2 (5 - 15 cm)	1.00
SRGF ² Layer 3 (15 - 30 cm)	0.42	SRGF ² Layer 4 (30 - 40 cm)	0.34
SRGF ² Layer 5 (40 - 50 cm)	0.23	SRGF ² Layer 6 (50 - 60 cm)	0.20
SRGF ² Layer 7 (60 - 70 cm)	0.18	SRGF ² Layer 8 (70 - 100 cm)	0.16
SRGF ² Layer 9 (100 - 125 cm)	0.04	SRGF ² Layer 10 (125 - 150 cm)	0.04
APSIM ³		APSIM ³	
y_hi_incr	0.011	x_hi_max_pot	1
tt_emergence	100	x_pp_end_of_juvenile	13
y_tt_end_of_juvenile	100	x_pp_floral_initiation	13
x_tt_floral_initiation	150	x_pp_flowering	13
x_tt_flowering	350	x_pp_start_grain_fill	13
y_tt_start_grain_fill	500	tt_end_grain_fill	20
tt_maturity	20	y_height	1500
shoot_lag	15	shoot_rate	1.4
KL Layer 1 (0 - 5 cm)	0.1	KL Layer 2 (5 - 15 cm)	0.1
KL Layer 3 (15 - 30 cm)	0.1	KL Layer 4 (30 - 40 cm)	0.06
KL Layer 5 (40 - 50 cm)	0.06	KL Layer 6 (50 - 60 cm)	0.02
KL Layer 7 (60 - 70 cm)	0.02	KL Layer 8 (70 - 100 cm)	0.01
KL Layer 9 (100 - 150 cm)	0.01		
MONICA		MONICA	
stage_temperature_sum Phase 1	140	stage_temperature_sum Phase 2	50
stage_temperature_sum Phase 3	555	stage_temperature_sum Phase 4	280
stage_temperature_sum Phase 5	910	stage_temperature_sum Phase 6	365

Table 6 – Summary of coefficients calibrated for each soybean crop model in the three phase of calibration processes

		(conclusion)	
Trait ¹	Value	Trait	Value
MONICA		MONICA	
stage_temperature_sum Phase 7	25	day_length_requirement ⁴	-13
base_day_lenght ⁴	-15.8	crop_specific_max_rooting_depth	75
slope PIRA	0.03	slope FW	0.05
slope LOND	0.05		
AQUACROP		AQUACROP	
Tb	10	TB	35
Kc _{max}	1.15	MERoot	1.1
SFR	20	MRWEup	0.024
MRWEbo	0.004	CDF	0
HIo	45	HIinc	4
HIvg	2	HIsc	5
S-E	85	S-MRD	998
S-SS	1580	S-M	1800
S-F	570	DF	356
CGC	0.01	CDC	0.014
GDD-BHI	1225		

¹The meaning of each coefficient is showed in Annex D; ²Mean values for three sites; ³Values of thermal time and photoperiod are 4 points to curve for each coefficients; ⁴Values are for phase from 2 to 6 (Annex D)

The aim of studies that use crop models can be the most diverse, including evaluation of environmental conditions, as current and future climate and soils, and management, as sowing date and cultivar. All models used in this study are able to predicted grain yield, which is the main response from the models, as well as, yield affect by sowing date and sites (BATTISTI; SENDELHAS, 2014) and climate change condition (GOUVÊA et al., 2009; ASSENG et al., 2013). Nendel et al. (2014) used the MONICA model to evaluate crop management, being sowing date, irrigation, crop rotation and N fertilizer option, to reduce the negative effect in the yield by climate change. Although a single model can be chosen, it is highly recommended to use an ensemble of crop models (MARTRE et al., 2015).

The results from the models also are used to estimate yield gap (VAN ITTERSUM et al., 2013; SENDELHAS et al., 2015), identifying limiting point in the crop growth. Deterministic models, as DSSAT, APSIM and MONICA, can be used to evaluation of physiological characteristics from cultivar or specie that can used to improve yield under different environmental conditions (BOOTE et al., 2011; SINGH et al., 2014). Crop rotation (MOHANTY et al., 2012), nitrogen balance (NENDEL et al., 2011) and crop water demand

(PAREDES et al., 2015) also can be evaluated using these crop models. This way, the crop model evaluated in this study are able to answer the aims for most agrometeorology analysis.

The model robustness is the capacity that model had to simulate crop growth and development in a specific condition. As discussed previous, it was possible to verified that all models were able to simulate soybean crop phases and yield efficiently. The main limitation was related with crop growth along crop cycle, as leaf area index and total above-ground biomass, and the harvest index. Martre et al. (2015) discussed that the inconsistency in others variables in the model can lead an good yield estimation, although in a wrong way, but is always necessary to improve the performance in the model to predicted these intermediate crop variable.

The transparency of model is important due to affect directed the capacity of user calibrate the model, define the model robustness, and identify if the model is able to attend their objectives. The model more simple is the FAO, where the yield is estimating based in a couple of equation and coefficients, with an expressive number of paper for soybean in Brazil (MONTEIRO; SENTELHAS, 2014; BATTISTI; SENTELHAS, 2014), being easily to find information about the model. The DSSAT is a complex model with a higher number of coefficients to describe cultivar development and growth, but is the model with higher number of paper about soybean, where can be find information about calibration process, definition of coefficients and processes simulated.

APSIM is a model with very similar complexity than DSSAT, with a good description of the model in the website (www.apsim.info), but specific to soybean, paper using and describing the model is poor. MONICA has the same condition than APSIM, where the codes to soybean are in development and there is no paper showing MONICA performance to soybean. The MONICA model description is made through of some paper and in the model website (<http://monica.agrosystem-models.com/>). AQUACROP has wide description of the model processes and how users can adjust the coefficients related with specie and cultivar, but with limited number of paper about soybean crop (RAES et al., 2012).

Other important points about the transparency are the support, interface and open codes source. The support is made to DSSAT and APSIM by developer and user through forum in the internet, where is possible to get answer for the more variables problem, and publication that describe the models and examples. MONICA and AQUACROP had the information available at website and publications, while for FAO, there is no support, due to be a simple model and AQUACROP be an update version of FAO.

For the interface of use, DSSAT has the better to calibrate and simulate, being easily to view the results and compare with observed data, but APSIM has similar interface, which had only the limitation about compare simulate and observed values. The models AQUACROP, MONICA and FAO need additional scripts made by the user to automation the simulation. The codes open is an important condition when additional simulation are require, but is highly recommended get in touch with developer when this is require.

2.4 Conclusions

Based in the results obtained in this study, it is possible to conclude that all models were able to simulated efficiently yield and crop phases to soybean for the region after calibrated the coefficients related with crop development, growth and related with soil. The models were able to capture different levels of yield in the sites of field experiment under rainfed and irrigated conditions. For the different phases of calibration, the most of models had worst performance in phase 1, using default values, and phase 2, calibrating only crop development, than phase 3, where all coefficients were adjusts. The performance of models in phase 1 and 2 were related with default coefficients in the model, where the models that had coefficients for the same maturity group than cultivar BRS 284 showed better performance, being DSSAT, APSIM and MONICA. It was observed that for all models was necessary to adjust coefficients related with soil that affect root water uptake, being a limiting point in the calibration that need to be analysis carefully. For this, it was adjust root growth and distribution in the soil for DSSAT, the maximum daily water uptake for APSIM, and maximum root depth for MONICA, AQUACROP and FAO, where the yield is higher sensitivity to these coefficients. For the results obtained in the simulation yield, using independent data, it was observed a poor performance, which occurred because of factors not consider by model, as diseases, and limited information about soil and climate specific from the sites of field experiment, committing model performance. This way, the choice of crop model to use in simulation of soybean growth can be done based in the capacity of model to attend the objective of study and accessible of information and knowledge of user to calibrate and use the model, once all model were able to simulate soybean yield after calibration. Other important point that can be consider is the use of the results from crop models ensemble, which had the best performance than the best single crop model.

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3 SENSITIVITY ANALYSIS OF FIVE SOYBEAN CROP GROWTH MODELS TO CLIMATE CHANGE

Abstract

The crop growth models have many uncertainties in the simulations due to the interactions in the processes simulated, parametrization and calibration, which can be investigated through sensitivity analysis. Based on that, the aim of this study was to evaluate the sensitivity of five crop models to systematic changes in climate for simulating soybean yield in Southern Brazil. The crop models used were: FAO-Agroecological Zone; AQUACROP; CSM – CROPGRO – Soybean; APSIM – Plant – Soybean; and MONICA. The simulations were performed for five sites in the Southern Brazil and sensitivity analysis considered changes of air temperature, [CO₂], rainfall and solar radiation in relation to the baseline climate independently and with interactions between them. The crop models simulated a reduction of attainable yield with temperature increase, which was due to shorter cycles. The different levels of response between models can be attributed to the approach and cardinal temperatures used for crop development. For rainfall, the most estimates showed an increase in the relative yield losses when changes from -15 to -30% were simulated. On the other hand, the models showed a positive yield relative response for rainfall increase. When solar radiation was increased, the positive yield responses were higher in Ponta Grossa, Campo Mourão and Avaré, while lower responses were observed in Cruz Alta and Dourados, which is associated with higher water deficit in these sites. The crop models had a reduction of relative yields gains when the [CO₂] was increased from 100 to 400 ppm, a consequence of the asymptotic soybean response to this atmospheric variable. The water deficit level and the approach used to photosynthesis simulation also affected the yield response to [CO₂]. Combining the climate scenarios and using models' ensemble, the yield was affected mainly by reduction of rainfall (increase of solar radiation), while temperature and [CO₂] interaction showed compensation effect on yield losses and gains. These results demonstrate that all models are sensitive to climate change despite some difference among them and that the use of models' ensemble can improve the confidence of yield simulations under future climate scenarios.

Keywords: *Glycine max* L.; Yield; Crop models ensemble; Models comparison; Uncertainty; Future climate scenarios

3.1 Introduction

Crop simulation models have been widely used in studies about crop management, such as sowing dates (BATTISTI; SENTELHAS, 2014), irrigation (DOGAN et al., 2007), nitrogen application (KASSIE et al., 2015) and farm management (NENDEL et al., 2014) for current climate. The models have been also used in the context of climate change to simulate yield impacts (ARAYA et al., 2015), adaptation measures (BOOTE, 2011) and best crop management (BAO et al., 2015). Thus, the simulations are important to evaluate different strategies to mitigate the impacts on yield.

However, the crop simulations present many uncertainties associated to the complexity of the model and to the interactions in the processes simulated, which are influenced by parametrization and calibration. These uncertainties can be computed by comparing model simulations (ASSENG et al., 2013; MARTRE et al., 2015) and evaluating the sensitivity of crop models to systematic changes in climate conditions (MARIN et al., 2015; PIRTIOJA et al., 2015; LI et al., 2015). Comparisons of these models help to understand the similarities and divergences between them (BASSU et al., 2014; LI et al., 2015; MARTRE et al., 2015), while systematic changes of weather variables help to understand how the model respond to climate conditions (PIRTIOJA et al., 2015), enabling to identify limitations in the crop models for climate change studies. Many studies have been performed about sensitivity analysis using systematic changes of climate and multiple crop models, as for wheat (PIRTIOJA et al., 2015), maize (BASSU et al., 2014; ARAYA et al., 2015), rice (LI et al., 2015) and sugarcane (MARIN et al., 2015). Otherwise, for soybean this kind of study is still restricted.

Southern Brazil is responsible for 45% of Brazilian soybean production (IBGE, 2015b). The main cause of yield gap in this region is the water deficit (SENTELHAS et al., 2015); while air temperature stresses are not a current problem, once the average air temperatures during soybean growing season remain between 17°C and 28°C, respectively for the coolest and hottest sites. For the future climate, the tendency is an increase in the temperature and [CO₂], while the projections for rainfall and solar radiation are not well defined yet (MARENGO et al., 2010; CHOU et al., 2012).

The crop yield response to climate change simulated by crop models is associated to the baseline climate, since locations with lower temperature will have positive yield response under higher temperatures and [CO₂], whereas warmer locations will have yield reduction, as observed for soybean (DERYNG et al., 2014), chickpea (SINGH et al., 2014) and rice (LI et al., 2015). The crop model parametrization can also lead to yield response variability (BASSU et al., 2014). Li et al. (2015) observed that differences in the models' approaches to reproduce temperature and [CO₂] effects on crop phenology, net primary production and spikelet fertility created a substantial variation in the grain yield.

Considering the importance of knowing the models performance under different climate conditions for studies of climate change and its impact on crop yield, the aims of this study were: (1) to simulate the soybean yield for the current climate conditions using five crop simulation models and compare the results with observed yield from official agencies to certify that crop models are able to capture yield variability due to climate in different regions

and crop seasons in Southern Brazil; (2) to evaluate the crop model sensitivity to systematic changes in air temperature, [CO₂], rainfall and solar radiation in the soybean growth and development using five crop simulation models; and (3) to evaluate the yield response for the interaction of air temperature and [CO₂] with rainfall and solar radiation using impact response surfaces.

3.2 Material and Methods

3.2.1 Sites, climate and soil data

Five sites were selected based on the breeding soybean zones (KASTER; FARIAS, 2012), the representatives of the grown area around each site (Figure 1 from chapter 1, pg. 13), and the climate cluster analysis in Southern Brazil. The cluster analysis was made by Ward method using the Euclidean distance, where the matrix have thirty sites in the line and in the columns the average of minimum and maximum air temperature, and total and standard deviation of rainfall during soybean growth season (Annex J). The selected sites were Cruz Alta, RS (28°37'48" S; 53°36'00" W; 472 m ASL), Ponta Grossa, PR (25°05'24" S; 50°09'36" W; 969 m ASL), Campo Mourão, PR (24°04'58" S; 52°21'36" W; 616 m ASL), Avaré, SP (23°04'48" S; 48°54'36" W; 813 m ASL), and Dourados, MS (22°16'12" S; 54°48'36" W; 408 m ASL).

The baseline climates were obtained for the period from 1961 to 2014, totalizing 53 growing seasons. Weather data used were maximum and minimum air temperature, rainfall, solar radiation, wind speed and relative humidity from Brazilian Meteorological Service (INMET), Agronomic Institute of Paraná (IAPAR) and Brazilian Agricultural Research Company (EMBRAPA). These data were used to create different climate series, based on systematic changes of air temperature, [CO₂], rainfall and solar radiation. The main current climate characteristics of each site are presented in Figure 1.

The soil type of each site was identified using the soil map from IBGE (2015a) and defining an area with a radius of 50 km from the point of the weather station with the software QGIS 2.6.1. The soil type was chosen according to the most representative one in the area. The data from RADAM Project (1974) were used to get information about sand, clay and silt contents, bulk density, drainage, pH, carbon and nitrogen contents for the corresponding type of soil, building the soil profile based on soils characteristics presented in Annex B. The soil

water holding capacity of each soil was estimated using pedotransfer functions developed by Reichert et al. (2009).

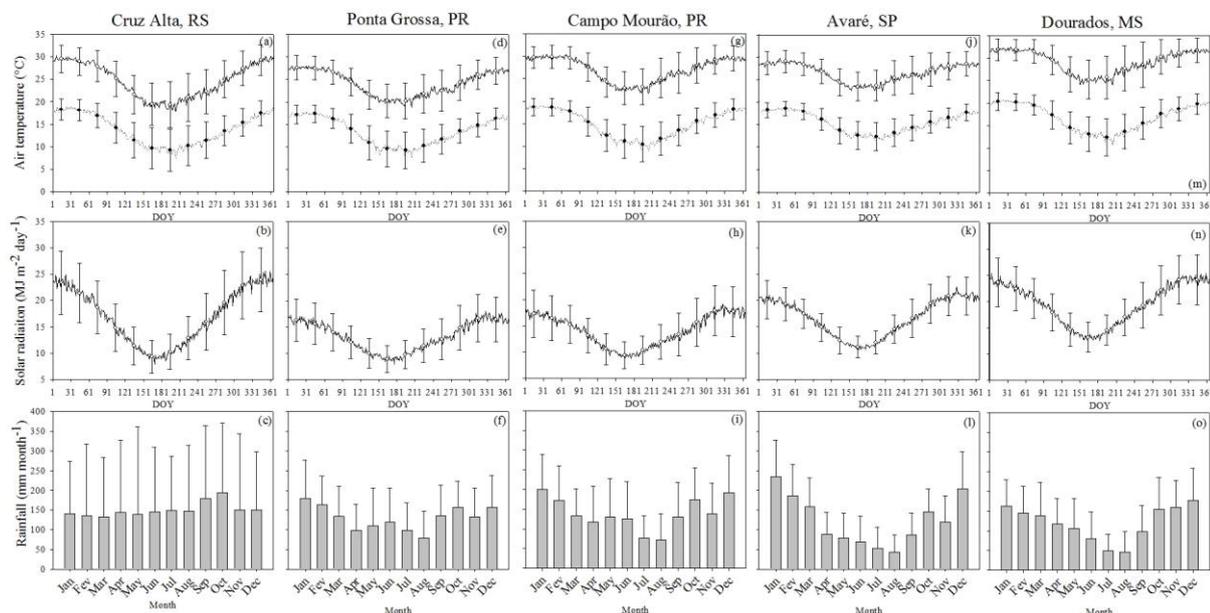


Figure 1 – Air temperature (a, d, g, j and m), solar radiation (b, e, h, k and n) and rainfall (c, f, i, l and o) in Cruz Alta, RS (a, b and c), Ponta Grossa, PR (d, e and f), Campo Mourão, PR (g, h and i), Avaré, SP (j, k and l), and Dourados, MS (m, n and o). For temperature and solar radiation, the lines are the daily average and points are the monthly average for the period 1961-2014, and bars indicate the standard deviation for each month. See Annex K for more details

In Southern Brazil, soybean is sowed between October and December, but the preferential date is in November (DO RIO et al., 2016). Based on that, the simulations were made using Nov 15th as the most representative sowing date. The simulation started 30 days previous sowing date, assuming that soil had recharged 75% of total water available for the crop. The cultivar parameters used in the models was from BRS 284, which is recommended for Southern Brazil, having a maturity group 6.5 (ALLIPRANDINI et al., 2009).

3.2.2 Crop simulation models

Soybean growth and development were simulated by five crop simulation models, as follows: FAO – Agroecological Zone (KASSAM, 1977; DOORENBOS; KASSAM, 1979; RAO et al., 1988), referred as FAO; FAO – AQUACROP v. 4.0 (STEDUTO et al., 2009; RAES et al., 2012), referred as AQUACROP; Model for Nitrogen and Carbon in Agroecosystems v. 2.11 (NENDEL et al., 2011), referred as MONICA; Crop System Model –

CROPGRO – Soybean v. 4.6.1 presented in the software Decision Support System for Agrotechnology Transfer (BOOTE et al., 1998, 2003; JONES et al., 2003), referred as DSSAT; and Agricultural Production Systems Simulator v. 7.7 (ROBERTSON; CARBERRY, 1998; KEATING et al., 2003; HOLZWORTH et al., 2014), referred as APSIM. The main characteristics of crop models are describe in Annex C and Appendix D.

The crop models were calibrated using observed results of intermittent growth (leaf area index, leaf, stem and pod dry mass, plant width and height) sampled six times along the crop cycle, variables obtained in the harvest (yield, harvest index, grain weight, grain and pod number) and timing of crop development (flowering, 1st pod, 1st seed and maturity). The data was collected during the 2013/2014 crop season in Frederico Westphalen, RS (27°21'38" S; 53°23'48" W; 540 m ASL) under rainfed conditions; Londrina, PR (23°11'34" S; 51°10'59" W; 634 m ASL) under rainfed and irrigated conditions; and Piracicaba, SP (22°42'14" S; 47°37'30" W; 569 m ASL) under rainfed and irrigated conditions. Five sowing dates were chosen at Frederico Westphalen and three at both Londrina and Piracicaba, between October and January, totaling 17 field experimental variations.

The cultivar used in all experiments was BRS 284, with maturity group 6.5, with an indeterminate growth habit, and classified as a conventional material. In the field experiments, fertilizer was applied to sustain crop growth without nutrient deficiency and was performed according to soil analysis, applying phosphorus and potassium and using rhizobium inoculation to improve nitrogen (N) fixation. The spacing between rows was between 0.45 and 0.50 m, with the plant population between 26 and 32 plants m⁻². Piracicaba had full irrigation, while in Londrina irrigation was gauged to supply an estimated 75% of maximum crop evapotranspiration.

3.2.3 Climate scenarios for sensitivity analysis

The sensitivity of crop model to the climate was evaluated changing air temperature, [CO₂], rainfall and solar radiation from baseline climate independently, changing one variable and fixing the baseline values of others. The air temperature was increased in 1.5, 3.0, 4.5 and 6.0°C, for minimum and maximum equally, preserving the baseline diurnal temperature range as adopted by Pirttioja et al. (2015). For rainfall and solar radiation the changes were of -30, -15, +15 and +30% in relation to the current conditions. The number of wet and dry days were not changed. The [CO₂] was evaluated using the current value of 380 ppm (NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION'S/EARTH SYSTEM RESEARCH

LABORATORY - NOAA/ESRL, 2015), and the following increased levels: 480, 580, 680 and 780 ppm. These values represent the projections simulated using the representative concentration pathways (RCPs) by IPCC (2014).

A second analysis was performed using impact response surface (PIRTTIOJA et al., 2015), which allows the interactions of changes in air temperature and CO₂ with rainfall and solar radiation. This analysis was done as a case study for Cruz Alta, RS, where 25 combined scenarios were created for temperature and [CO₂]. For each combination of temperature and [CO₂] changes in rainfall and solar radiation were also included, assuming that changes in rainfall affect the solar radiation inversely, due to presence of clouds (Table 1).

Table 1 – Combined climate scenarios for air temperature (T) and CO₂ concentration ([CO₂]) and for rainfall (R) and solar radiation (SR)

Climate Scenario	ΔT (°C)	$\Delta [CO_2]$ (ppm)	Climate Scenario	ΔR (%)	ΔSR (%)
T-CO ₂ 1	0	380	R-SR1	-30	+30
T-CO ₂ 2	+1.5	480	R-SR2	-15	+15
T-CO ₂ 3	+3.0	580	R-SR3	0	0
T-CO ₂ 4	+4.5	680	R-SR4	+15	-15
T-CO ₂ 5	+6.0	780	R-SR5	+30	-30

3.2.4 Data analysis

Yield inter-annual variability (1961-2014) and crop models were evaluated for the five sites considering the baseline climate. The inter-annual variability was analyzed by plotting the simulated attainable yield by the models against harvest year. The simulated yields from the ensemble of the models (an average of them) were also plotted, as well as, the percentil of 5 and 95% from all of them. It was also added in the analysis the observed yield of each site, obtained from CONAB (2015), from 1977 to 1989, and from IBGE (2015b), from 1990 to 2014, with the technological tendency removed, as recommended by Heinemann and Sentelhas (2011). These actual soybean yields represent the average from farmers for each crop season considering different crop cycles and sowing dates.

For independent sensitivity analysis, the following variables were evaluated: potential and attainable yields; maximum and actual crop evapotranspirations; and days after sowing to beginning of flowering and maturity. The responses from the crop models for these variables were compute as relative response by unit of change in relation to the climate variable, being by °C for air temperature, ppm for [CO₂], and percentage for rainfall and solar radiation. For assessment of the combined impact of climate variations on yield, response surface analyzes

considering changes of air temperature and [CO₂] (x-axis) and rainfall and solar radiation (y-axis) were used, with soybean attainable yield response being represented by the contour lines in percentage of change (PIRTTIOJA et al., 2015). The same analysis was performed for average yield from the ensemble of the five crop models.

3.3 Results and Discussions

3.3.1 Crop model performance

In order to be used for different agrometeorological purposes, the crop simulation models need to be able to simulate yield in different environmental conditions. For that, they must be enough calibrated for producing reliable results in terms of growth, development and yield. The models used in this study showed similar performance between them for estimating yield, with root mean square errors (RMSE) lower than 650 kg ha⁻¹ (Table 2) and d index over 0.90. The dates of beginning of flowering (R1) and maturity (R7) were also well estimated by crop models (Table 2), with RMSE of less than 4.2 days for R1 and less than 6.5 days for R7, showing to be suitable for simulating crop growth and development accurately.

Table 2 – Crop simulation models performance for soybean grain yield, flowering and maturity after calibration using data from field experiments

Crop model	Grain Yield			Flowering (R1)			Maturity (R7)		
	Mean	RMSE ³	d ⁴	Mean	RMSE ³	d ⁴	Mean	RMSE ³	d ⁴
	Kg ha ⁻¹			DAS ⁵			DAS ⁵		
Measured	2883	-	-	41	-	-	107	-	-
² FAO	3006	650.0	0.91	-	-	-	-	-	-
AQUACROP	3047	536.1	0.91	42	4.1	0.79	105	6.0	0.84
DSSAT	2948	548.3	0.93	42	3.0	0.87	107	4.4	0.94
APSIM	3038	549.7	0.90	41	4.2	0.81	108	5.1	0.91
MONICA	2850	538.9	0.92	42	4.0	0.80	109	6.5	0.84

¹Measured data is based on results from seventeen field experiments; ²FAO does not simulate crop development phases; ³RMSE = root mean square error; ⁴d = Willmott agreement index; ⁵DAS = Days after sowing

3.3.2 Baseline yields

The soybean yield estimated by the five crop models and the ensemble of them in comparison to observed yield are shown in Figure 2. A high yield variation was observed between models for all sites along the 53 years of simulation. These differences were caused by the interactions of models characteristics and local climate, which is common, as observed

by Pirttioja et al. (2015) when employed 26 crop models for wheat, as well as by Li et al. (2015) for rice and by Kassie et al. (2015) for maize. The sensitivity of crop models to climate change is dependent of current climate (DERYNG et al., 2014), and models' structure and parametrization (BASSU et al., 2014; SOLTANI; SINCLAIR et al., 2015), which introduce uncertainty into crop yield estimates even for the present-day conditions (WHITE et al., 2011).

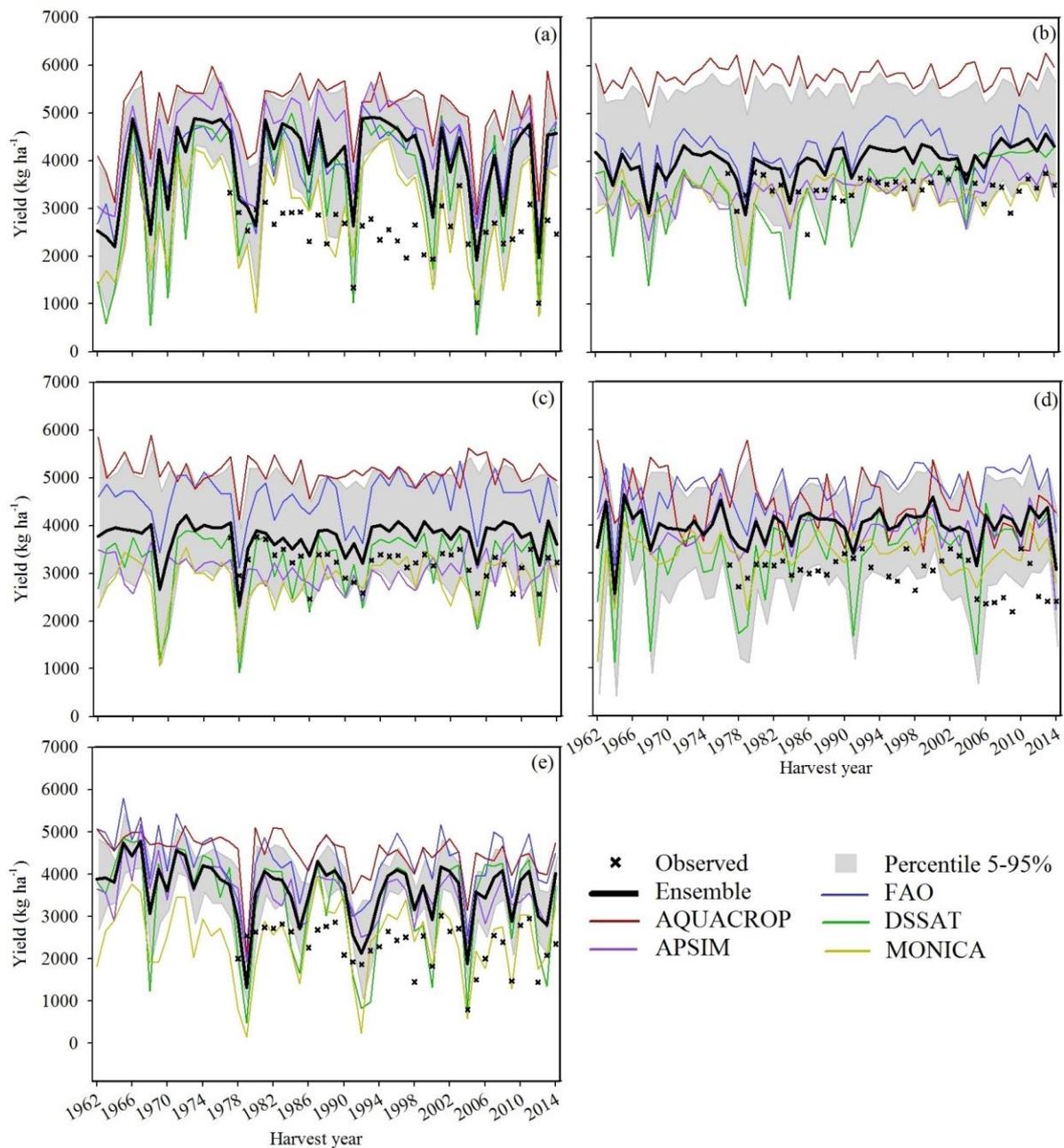


Figure 2 – Soybean grain yield for five sites in Southern Brazil: Cruz Alta (a), Ponta Grossa (b), Campo Mourão (c), Avaré (d) and Dourados (e). Lines correspond to the estimated yield by the five crop simulation models and their ensemble and symbol (x) to the average observed yield in the field, for the period of 1962 to 2014

The attainable yield estimated by the models were, in general, higher than observed yield, which is an average of all farmers, with many crop cycles, sowing dates and soils, and other conditions that can lead to yield gap (SENTELHAS et al., 2015). Although the simulated yields are above observed, showing different levels between models, it is possible to observe that the models were able to capture the same tendency of observed yield along the crop seasons. Pirttioja et al. (2015) observed that when using normalized yields by the mean simulated yield of each crop model, the models were able to simulate the environmental effects on yield variability.

3.3.3 Temperature responses

The crop models simulated a reduction in the attainable yield in most cases when air temperature was increased (Table 3). The reduction of yield is attributed mainly to the shorter crop cycle, as also observed by Bassu et al. (2014) and Kumagai and Sameshima (2014). The only exception was for FAO model that had a slight positive response, between 2 e 21 kg ha⁻¹ °C⁻¹ in some specific conditions (site x temperature increase) (Table 3). This happened because this model considers a constant crop cycle for all climate scenarios. The AQUACROP and APSIM presented reductions in the relative response with air temperature increase for all sites, reaching, respectively, an absolute yield change of -1890 and -1440 kg ha⁻¹ for Ponta Grossa, PR, the coldest assessed site (Annex K), when applied an increase of 6 °C.

The models' parametrization in relation to the crop cycle is the main aspect that affect the relative yield response to air temperature. For AQUACROP, the higher relative response under lower increased temperature is due to the positive relationship between development rate and temperatures between 10 and 35°C, while above 35°C, values reached with 6°C increase, such relationship is negative (RAES et al., 2012). Similar effect occurred when yields were simulated with APSIM, which uses a positive linear development rate between 10°C and 30°C, and negative between 30°C and 40°C (APSIM, 2015).

DSSAT model presented a similar response for the four levels of temperature increase, except for the warmest site (Dourados, Annex K), where the relative response to air temperature increase, achieved an absolute reduction of 1878 kg ha⁻¹ under +6 °C. This model had a similar response for all scenarios since maximum photosynthesis rate has a wider range of air temperature, from 21 to 36 °C, and crop cycle was less reduced when compare to other models, once it uses a higher upper limit temperature (45°C) (BOOTE et al., 1998). The

relative yield response of MONICA to increasing air temperature (Table 3) also showed a reduction of 223 to 314 kg ha⁻¹ °C⁻¹, caused by shorter crop cycle. It was caused by the absence of an upper limit temperature, which makes the model more sensitive to temperature changes (MONICA, 2015).

Table 3 – Relative soybean attainable yield response in relation to the baseline for changes in air temperature, using five crop simulation models in different locations of Southern Brazil

Crop Model	Baseline (kg ha ⁻¹)	Relative response (kg ha ⁻¹ °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
Cruz Alta					
FAO	3970	-17	-22	-30	-41
AQUACROP	5039	-388	-330	-297	-275
DSSAT	3516	-252	-258	-262	-263
APSIM	4468	-294	-269	-237	-206
MONICA	2918	-223	-233	-261	-267
Ponta Grossa					
FAO	4273	2	4	0	-9
AQUACROP	5800	-389	-363	-336	-315
DSSAT	3325	-216	-222	-222	-217
APSIM	3360	-370	-342	-290	-240
MONICA	3300	-247	-272	-282	-289
Campo Mourão					
FAO	4584	21	10	-5	-21
AQUACROP	5139	-293	-273	-258	-234
DSSAT	3222	-211	-210	-208	-209
APSIM	3032	-290	-216	-168	-141
MONICA	2836	-272	-272	-285	-290
Avaré					
FAO	4720	18	19	10	-3
AQUACROP	4444	-289	-243	-219	-199
DSSAT	3403	-188	-187	-178	-170
APSIM	3897	-410	-338	-270	-214
MONICA	3368	-278	-287	-291	-296
Dourados					
FAO	4306	-32	-48	-64	-82
AQUACROP	4501	-263	-235	-210	-189
DSSAT	3342	-253	-265	-286	-313
APSIM	3550	-188	-143	-114	-100
MONICA	2471	-288	-307	-314	-304

As observed, the relative yield response to temperature is a resultant of the interactions between model, site and climate scenarios (ASSENG et al., 2013; PIRTIOJA et al., 2015), which affect other crop variables estimates by the models (MARTRE et al., 2015). For potential yield (Table 4), the only model with positive response to temperature increase was FAO, while the others simulated yield reductions. Such reductions are caused by shorter crop cycles that lead to less solar radiation interception and, consequently, to less photosynthesis (SPEHAR et al., 2015).

Changes in temperature will also affect maximum and actual crop evapotranspirations changing the water deficit to the crops along the cycle. However, reduction in total maximum crop evapotranspiration can occur, as simulated by AQUACROP and MONICA, caused by shorter cycle. On the other hand, FAO, DSSAT and APSIM simulated an increase of this variable. For total actual crop evapotranspiration, FAO and DSSAT simulated increase of this variable, although in lower rate than maximum crop evapotranspiration (Table 4), increasing the relative water deficit

3.3.4 Rainfall responses

The models had a clearly tendency of yield decreased when rainfall was reduce in 15 and 30% for all sites, with opposite trend with rainfall increase (Data no showed). The higher yield losses occurred in Dourados, reaching 1410 and 1320 kg ha⁻¹, respectively, for DSSAT and MONICA models. This site and these models also had the highest yield gains with rainfall increase, respectively 23 and 21 kg ha⁻¹ percent⁻¹. These results can be explained by the higher frequency of water deficit during soybean growing season in this site (FIETZ; RANGEL, 2008; SENTELHAS et al., 2015).

Most simulations showed a higher relative yield loss when rainfall was reduced by 15 and 30%, caused by crop response to water deficit. Candogan et al. (2013) showed that soybean yield was linear reduced when crop evapotranspiration was below 500 mm during the cycle. On the other hand, the models showed a yield improvement when rainfall was increased by 15% and 30% (Data no showed). The changes in rainfall were applied only to water amount, with no change in the number of wet days, which increased simulated runoff and deep drainage. If from one side it can be considered a limitation of this kind of analysis, from the other these results show the importance of improving the soil management, under such scenarios, to reduce runoff (FRANCHINI et al., 2009), such as no-tillage (BERTOL et al., 2008) and contour sowing and strip cropping (BORGES et al., 2014).

Table 4 – Relative soybean potential yield, actual (ETa) and maximum (ETm) crop evapotranspirations, and days after sowing for flowering (R1) and maturity (R7) in relation to the baseline for changes in air temperature, using five crop simulation models in Cruz Alta, RS

Crop Model	Baseline (kg ha ⁻¹)	Relative Potential Yield Response (kg ha ⁻¹ °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
FAO	6218	76	68	56	38
AQUACROP	5520	-317	-290	-267	-244
DSSAT	4744	-108	-138	-155	-176
APSIM	5418	-167	-152	-143	-141
MONICA	3835	-312	-316	-343	-346

Crop Model	Baseline (mm cycle ⁻¹)	Relative ETa Response (mm °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
FAO	376	6	6	6	6
AQUACROP	554	-20	-18	-16	-14
DSSAT	624	1	1	2	4
APSIM	568	-8	-5	-3	0
MONICA	528	-14	-12	-10	-9

Crop Model	Baseline (mm cycle ⁻¹)	Relative ETm Response (mm °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
FAO	547	17	17	17	18
AQUACROP	602	-13	-12	-10	-9
DSSAT	741	11	12	13	15
APSIM	777	11	14	15	15
MONICA	535	-14	-13	-11	-9

Crop Model	Baseline (DAS ¹)	Relative R1 Response (days °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
FAO ¹	-	-	-	-	-
AQUACROP	45	-2.89	-2.62	-2.36	-2.13
DSSAT	53	-2.49	-2.00	-1.57	-1.14
APSIM	30	-1.38	-1.18	-0.94	-0.70
MONICA	45	-2.43	-2.23	-2.03	-1.86

Crop Model	Baseline (DAS ¹)	Relative R7 Response (days °C ⁻¹)			
		1.5°C	3.0°C	4.5°C	6.0°C
FAO ¹	-	-	-	-	-
AQUACROP	137	-11.06	-9.20	-7.88	-7.06
DSSAT	120	-2.68	-2.19	-1.63	-1.09
APSIM	123	-4.35	-3.40	-2.49	-1.62
MONICA	119	-5.02	-4.21	-3.54	-3.01

¹DAS: days after sowing

DSSAT and MONICA were the models that presented the highest yield changes with rainfall variation, similar tendency observed in the analysis of the baseline (Figure 2), with

these models being more sensitive to dry years than others. The APSIM and AQUACROP showed the lower changes in yield response. APSIM when not properly parameterized for root growth can lead to higher water availability for crop uptake. Similarly, AQUACROP model allows higher water availability for the crop, resulting in higher yield. The FAO model had intermediate yield changes, demonstrating that the simple approach used for water balance calculation (THORNTHWAITE; MATHER, 1955) was able to represent more accurately water availability for soybean. The yield changes are mainly affect by actual crop evapotranspiration simulated by the crop models according to each scenario. Figure 3 shows the higher reduction and increase in actual crop evapotranspiration, respectively, of -142 mm for -30% of rainfall and 41 mm for +30% of rainfall, simulated by model MONICA model in Dourados.

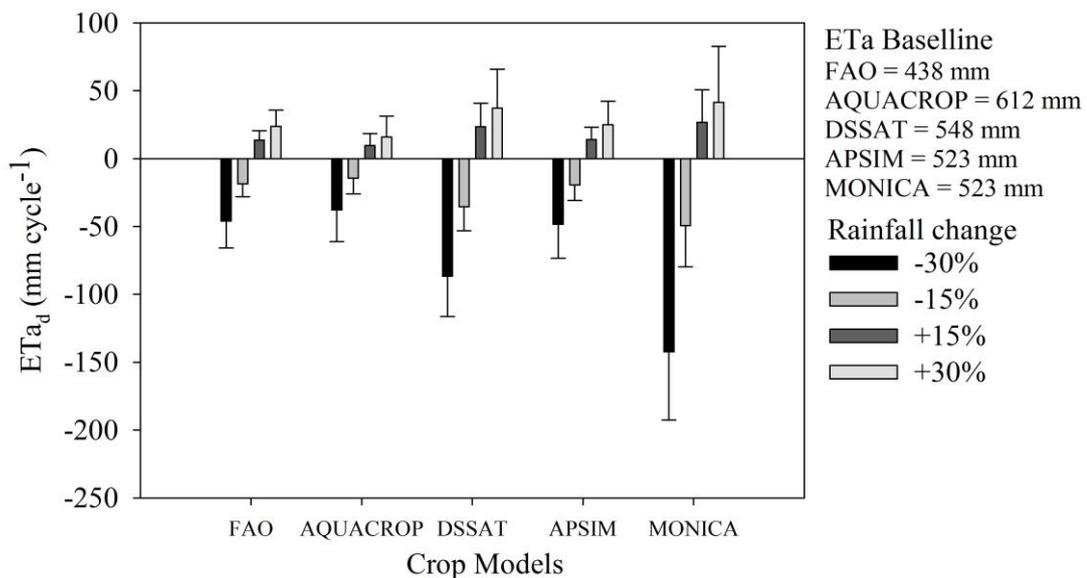


Figure 3 – Actual crop evapotranspiration difference (ETa_d) from the baseline, simulated by five crop simulation models with changes of -30, -15, +15 and +30% in the current values of rainfall for Dourados, MS. The bars indicate the standard deviation

3.3.5 Solar radiation responses

The highest relative yield response for solar radiation (SR) was observed when APSIM model was used, reaching $-61 \text{ kg ha}^{-1} \text{ percent}^{-1}$ of change for the scenario -30% in Avaré, while the best response was $+23 \text{ kg ha}^{-1} \text{ percent}^{-1}$ for both +15 and +30% scenarios, in Campo Mourão (Table 5). FAO and DSSAT models presented a negative response of attainable yield with SR reduction, but with no more than $15 \text{ kg ha}^{-1} \text{ percent}^{-1}$ for all scenarios (Table 5). When SR was increased, the sites of Ponta Grossa, Campo Mourão, and Avaré

(with lower water deficit) had positive yield responses simulated by most of crop models, while in Cruz Alta and Dourados (with higher water deficit) negative yield responses were observed for most cases (Table 5). These results show the importance of the balance between crop photosynthesis and water deficit, related with solar radiation, in order to identify the true effect of climate change and variability on soybean yield (REICOSKY et al., 1994; CANDOGAN et al., 2013).

Table 5 – Relative soybean attainable yield response in relation to the baseline for changes in solar radiation, using five crop simulation models in different locations of Southern Brazil

Crop Model	Baseline (kg ha ⁻¹)	Relativity response (kg ha ⁻¹ percent ⁻¹)			
		-30%	-15%	+15%	+30%
Cruz Alta					
FAO	3970	-2	-1	-1	-3
AQUACROP	5039	8	11	-23	-23
DSSAT	3516	-7	0	-12	-15
APSIM	4468	-36	-37	7	8
MONICA	2918	-10	-9	6	4
Ponta Grossa					
FAO	4273	-6	-6	5	3
AQUACROP	5800	2	3	-4	-6
DSSAT	3325	-25	-22	13	8
APSIM	3360	-59	-58	22	21
MONICA	3300	-20	-19	17	16
Campo Mourão					
FAO	4584	-8	-7	5	2
AQUACROP	5139	-1	-1	-2	-3
DSSAT	3222	-21	-17	9	6
APSIM	3032	-57	-59	23	23
MONICA	2836	-15	-13	12	11
Avaré					
FAO	4720	-10	-9	7	6
AQUACROP	4444	-10	-10	5	4
DSSAT	3403	-22	-16	7	3
APSIM	3897	-61	-58	19	19
MONICA	3368	-21	-20	13	12
Dourados					
FAO	4306	-3	-2	0	-2
AQUACROP	4501	4	5	-10	-14
DSSAT	3342	-10	-3	-9	-14
APSIM	3550	-48	-43	9	9
MONICA	2471	-9	-4	5	4

3.3.6 CO₂ responses

The crop models had a reduction of relative yield gains when the [CO₂] was increase in relation to the present scenario, between +100 and +400 ppm (Table 6), conditions associated with the asymptotic response of photosynthesis increase to [CO₂] (ALAGARSWAMY et al., 2006). Using the highest (AQUACROP) and lowest (MONICA) rates of relative response from Cruz Alta (Table 6), and applying the [CO₂] increase from difference studies, it is possible to observed similar tendency of soybean yields. Morgan et al. (2005), evaluating [CO₂] of 370 and 550 ppm, obtained soybean yield increase of 15%, while in the present study the response was between 11 and 26% using the relative response rate for 580 ppm. Hao et al. (2014) found yield gains between 26 and 31% with [CO₂] of 550 ppm in relation the baseline (415 ppm), while in our study crop simulation models generated a yield increase between 9 and 20%. With higher change, from 400 to 700 ppm, Heinemann et al. (2006) observed an increase of 7.5%, against 17 to 40% in present study.

The model with higher yield response to [CO₂] was AQUACROP, which reached a relative response of 10.09 kg ha⁻¹ ppm⁻¹ for the scenario with increase of 100 ppm in Ponta Grossa (Table 6). Otherwise, MONICA was the model with lower response in comparison with the other crop models used in this study. These results are associated with yield level simulated by each model and the sensitivity of them and the crop to water deficit. When the water deficit is more intense, the benefit from CO₂ fertilization can be reduced by water deficit, while in good conditions, such as less water deficit simulated by AQUACROP, the response to CO₂ fertilization will be higher (AINSWORTH; LONG, 2005; LI et al., 2013).

Other physiological process simulated by the crop models (except FAO) was the lower rate of transpiration (Data not showed), due to the reduction on stomatal conductance stimulated by a higher [CO₂] in the atmosphere and, consequently, in the intercellular space (BOOTE et al., 1997). Although crop models consider this effect, the relative responses to that were nearly constant between the models, mainly due to the lack of experimental data to describe this process or coefficients to be used in the simulations (LEAKEY et al., 2006).

3.3.7 Combined effects of climate scenarios on yield

The models had difference patterns and levels of relative attainable yield response to combined effects of climate change (Figure 4). Analyzing attainable yield with no change in precipitation and solar radiation (R-SR3), FAO model had a gradual yield increase, reaching

+20% for scenario T-CO₂5 (Figure 4a). AQUACROP and APSIM showed a compensatory effect between increase of temperature and CO₂ (Figure 4b and 4d), as also observed by Koti et al. (2007) and Deryng et al. (2014). For DSSAT model, a compensatory effect was also observed till T-CO₂3, however for T-CO₂4 and T-CO₂5 yield reductions occurred (Figure 4c). MONICA model was the only one with gradual reduction of yield with air temperature and CO₂ increases, till -26% for scenario T-CO₂5 (Figure 4e).

Table 6 – Relative soybean attainable yield response in relation to the baseline for changes in [CO₂], using five crop simulation models in different locations of Southern Brazil

Crop Model	Baseline (kg ha ⁻¹)	Relativity response (kg ha ⁻¹ ppm ⁻¹)			
		+100	+200	+300	+400
Cruz Alta					
FAO	3970	4.62	3.49	2.91	2.53
AQUACROP	5039	9.24	7.36	6.72	6.15
DSSAT	3516	4.97	4.36	3.88	3.50
APSIM	4468	4.29	3.96	3.69	3.46
MONICA	2918	2.13	1.90	1.67	1.51
Ponta Grossa					
FAO	4273	4.85	3.66	3.05	2.64
AQUACROP	5800	10.09	7.95	7.22	6.54
DSSAT	3325	4.29	3.75	3.34	3.02
APSIM	3360	4.11	3.61	3.23	2.92
MONICA	3300	2.53	2.13	1.83	1.60
Campo Mourão					
FAO	4584	5.42	4.09	3.42	2.96
AQUACROP	5139	8.85	6.94	6.28	5.66
DSSAT	3222	4.46	3.91	3.49	3.16
APSIM	3032	4.39	3.85	3.45	3.13
MONICA	2836	2.87	2.29	1.97	1.80
Avaré					
FAO	4720	5.40	4.08	3.40	2.95
AQUACROP	4444	7.19	5.53	4.94	4.41
DSSAT	3403	4.81	4.19	3.75	3.38
APSIM	3897	4.62	4.08	3.69	3.36
MONICA	3368	3.21	2.63	2.17	1.85
Dourados					
FAO	4306	5.41	4.09	3.42	2.97
AQUACROP	4501	7.97	6.31	5.73	5.19
DSSAT	3342	4.76	4.21	3.81	3.50
APSIM	3550	4.40	4.04	3.78	3.55
MONICA	2471	3.99	3.08	2.55	2.20

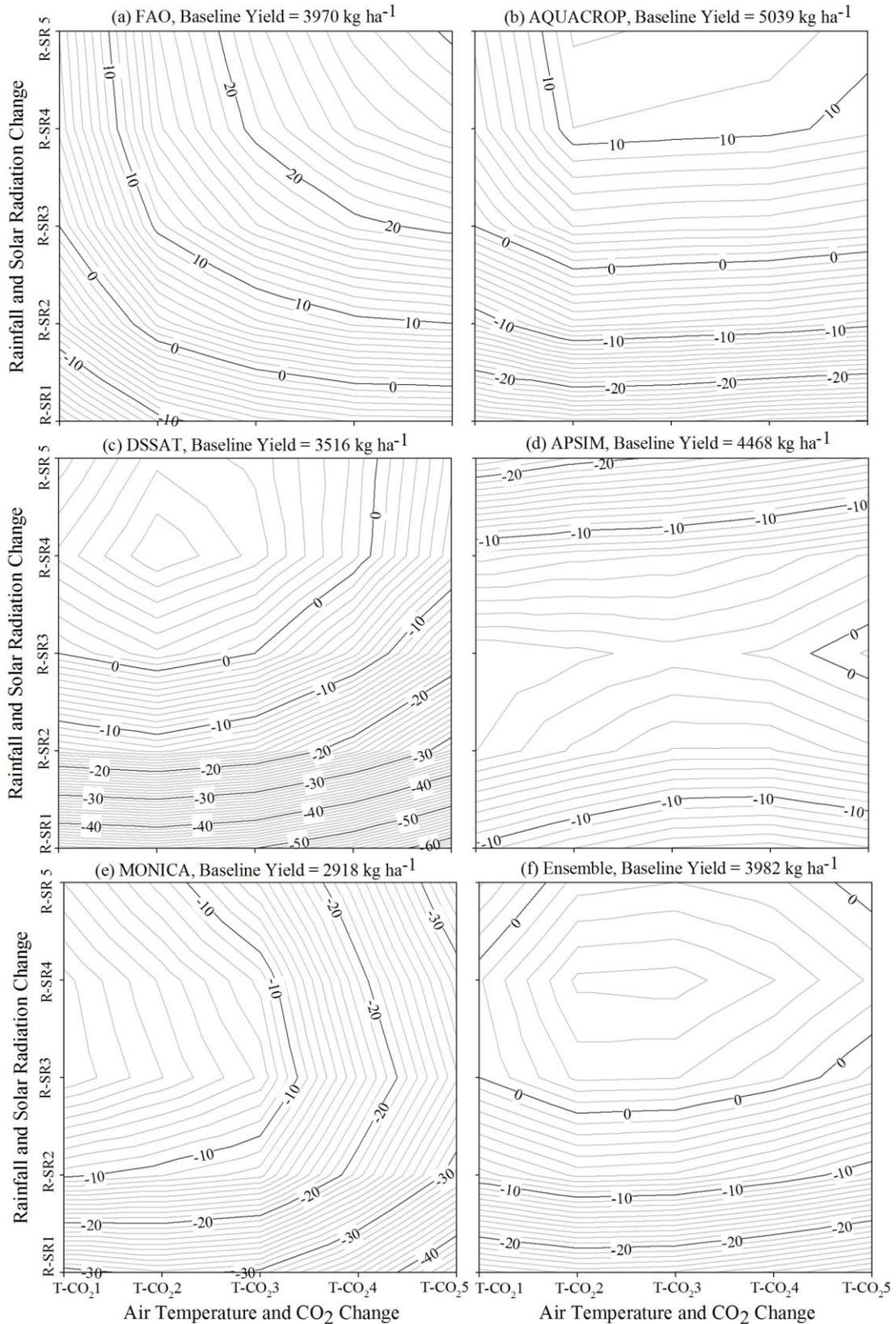


Figure 4 – Percentage of attainable soybean yield change, estimated by five crop simulation models and with their ensemble (mean), in relation to variation of air temperature (T), [CO₂], solar radiation (SR) and rainfall (R) in Cruz Alta, RS. The results are the average of 53 crops seasons. Scenarios are describe in Table 2

FAO model simulated a yield reduction when rainfall was reduced and solar radiation was increased (R-SR1 and R-SR2), whereas for the opposite condition, these factors had low influence (Figure 4a). Similar tendency was observed for AQUACROP simulations, but with yield increase when a rainfall increase of 15% and a solar radiation reduction of the same level (R-SR4) were simulated (Figure 4b). DSSAT model showed a yield reduction with less rainfall and more solar radiation (R-SR1 and R-SR2), and a yield increase till scenario T-CO₂4 (Figure 4c). For APSIM model, a negative yield response occurred for all scenarios of R-SR in relation to the baseline (Figure 4d). MONICA model was more influenced by rainfall and solar radiation (R-RS) till scenario T-CO₂3, with yield reduction with less rainfall. For the other scenarios, temperature and [CO₂] had more control on yields (Figure 4e).

The models' ensemble did not present a clearly tendency of yield change ($\pm 5\%$) with increase of air temperature and [CO₂] when combined with no change or increase of rainfall and reduction of solar radiation (R-SR3, R-SR4 and R-SR5) (Figure 4f). These results show that increase of [CO₂] can compensate the losses caused by higher air temperature by greater carbonic gas assimilation. In this context, more investigations are required for a better understanding of soybean response to higher [CO₂], once photosynthesis cannot be kept high due to rubisco consumption (WALTER et al., 2015). On the other hand, when reduction of rainfall and increase of solar radiation (R-RS1 and R-RS2) was used for yield simulation with the models' ensemble (Figure 4f), the results showed an attainable yield reduction of 29%.

DSSAT and MONICA models presented the highest standard deviations, reaching respectively, 1409 and 1085 kg ha⁻¹ for the baseline conditions (Figure 5) in relation to the simulation done. FAO, AQUACROP, and APSIM models and the models' ensemble had standard deviation ranging between 729 and 974 kg ha⁻¹ (Figure 5). The main responsible for yield variability in the simulations with the different scenarios were rainfall and solar radiation, as observed for AQUACROP model, which produced yield standard deviation of 130% with a reduction of 30% in rainfall and an increase of 30% in solar radiation. Pirttioja et al. (2015) and Asseng et al. (2013) also observed different levels of standard deviation between crop models, sites and scenarios used for simulating crop performance under future climate scenarios.

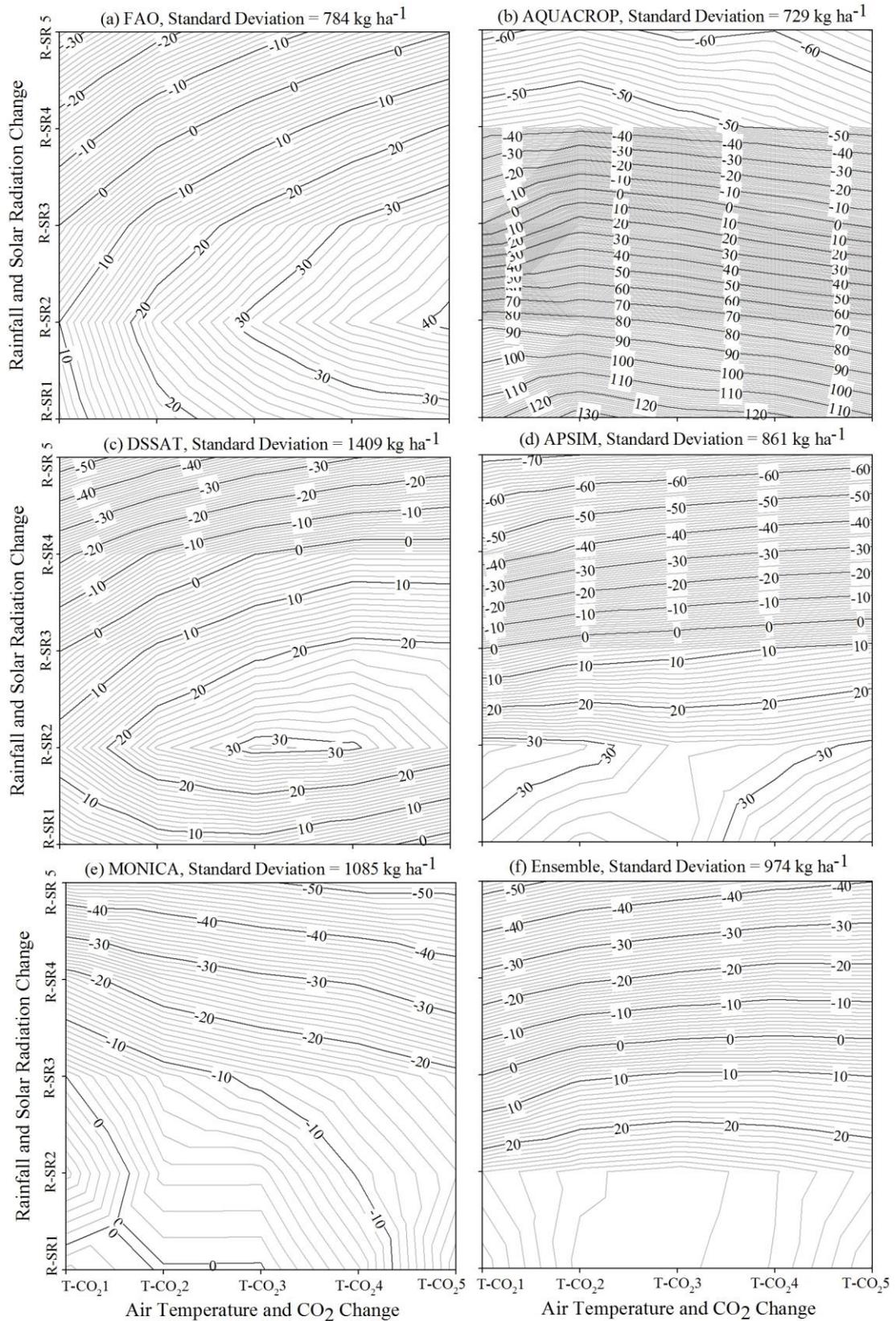


Figure 5 – Percentage of soybean yield standard deviation change estimated by five crop simulation models and with their ensemble (mean) in relation to variation of air temperature, [CO₂], solar radiation and rainfall in Cruz Alta, RS. The results are the average of 53 crops seasons. Scenarios are describe in Table 2

3.4 Conclusions

Crop models were able to simulate different soybean yield levels in the assessed sites, following observed yield inter-annual variability along the crop seasons. The models were sensitivity to changes in air temperature, [CO₂], solar radiation and rainfall. In most cases, crop models simulated a reduction of soybean yield when the air temperature was increased, what was caused by a shorter crop cycle in relation to the baseline data. The level of soybean yield change depended on the crop model approach used to estimate crop development, mainly associated to the cardinal temperatures considered by each of them. When rainfall was changed, the models simulated higher yield reductions due to lower rainfall amount than the yield increase with more rainfall. This occurred mainly because the increase on rainfall amount with no change in wet days just was enough to increase runoff and drainage, with low effect on yield. Solar radiation changes affect soybean yields in different ways depending on the crop models. The yield response to solar radiation was controlled basically by the water deficit. Even considering the increase of potential yield with more solar energy, it also increase maximum crop evapotranspiration, resulting in more water deficit. The relative yield gains were higher under lower [CO₂] increase (+100 ppm) than under higher increase (+400 ppm), for all models, which was a consequence of the similar asymptotic response curve that all models use for CO₂ assimilation. The yield responses were higher when simulated by models that compute less crop water deficit, once this process can penalize yield and cancel the benefits brought by higher [CO₂] for C₃ crops. One limiting aspect for the majority of crop models was to the secondary effect of [CO₂] on stomatal conductance and consequently on transpiration. Although they can simulate that, the responses are low and, probably, do not represent what happens in the field. So, it requires more attention from modelers in order to improve models for simulating more accurately the future scenarios of [CO₂]. Finally, combining all climate changes, the models showed that the benefits of increased [CO₂] for soybean yield can compensate the negative effect of increased air temperature; therefore, the present results show that soybean yield was more affected by associated changes on rainfall and solar radiation.

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4 ASSESSMENT OF SOYBEAN YIELD WITH ALTERED WATER-RELATED GENETIC IMPROVEMENT TRAITS UNDER CLIMATE CHANGE

Abstract

The water deficit is a major factor responsible for the soybean yield gap in Southern Brazil and tends to increase under climate change. One alternative to reduce yield gap attributed to water deficit is the selection of soybean cultivars with altered water-related traits associated with drought tolerance. Thus, the aim of this study was to assess soybean adaptive traits to water deficit that can improve yield under current and future climate to provide guidelines for soybean cultivars breeding in Southern Brazil. The CSM-CROPGRO-Soybean crop model was calibrated using growth and phenological data from Southern Brazil, where soybean was grown under different water levels and sowing dates. The following soybean traits were manipulated: deeper root depth in the soil profile; maximum fraction of shoot dry matter diverted to root growth under water stress; early reduction of transpiration under mild stress; transpiration limited as a function of vapor pressure deficit; N₂ fixation drought tolerance; and reduced acceleration of grain filling period in response to water deficit. The yields were predicted for standard and altered traits using climate data for the current (1961-2014) and future (middle-century) scenarios. The future climate included increased [CO₂] and air temperature. The traits with greater improvement in total production for the region were deeper rooting profile, with increase in total production of 3.3 % and 4.0 %, respectively for the current and future climates, followed by transpiration limited as a function of vapor pressure deficit and grain filling period. The maximum fraction of shoot dry matter diverted to root and N₂ fixation drought tolerance increased production by less than 1.0 % for both scenarios, while early reduction of transpiration had a small positive result only for the future conditions. When the better traits were combined, the simulated production increased about 9.0 % in the future climate. For benefitting soybean breeding programs, traits that create a deeper and greater root profile in the soil, reduce transpiration under water deficit more than photosynthesis, create tolerance of nitrogen fixation to drought, and reduce acceleration of grain filling period under water deficit showed positive effects and should be included alone or together in new soybean cultivars for Southern Brazil.

Keywords: Water deficit; Crop model; Adaptation to drought; Soybean breeding

4.1 Introduction

Brazil is one the most important soybean producers in the world, supplying around 30% of this commodity in the global market in 2013 (FAO, 2015), while Southern Brazil, the five-state region of this study, contribute for almost 45% of the Brazilian soybean production in the same year (IBGE, 2015b). Soybean yield is highly dependent on weather conditions, as most of the soybean areas in the country is grown as rainfed crop. Thus, drought in the present and future climates are of great concern for the soybean production in this region.

In southern Brazil, the larger soybean yield gaps are caused by droughts (SENTELHAS et al., 2015). Under climate change, water deficit may be more frequent and

intense, especially in the tropical and subtropical regions due to increased air temperature and altered rainfall pattern (LI et al., 2013; IPCC, 2015), which will require adaptation measures. In this way, White et al. (2011) suggested that soybean cultivars should be adapted to rising CO₂, heat stress and water deficit, resulting in a better water and nutrient use efficiency.

The crop adaptations for adverse climate conditions, as water deficit and extreme temperatures, are important to reduce the yield gaps and improve yields. A better cultivar can be developed by adjusting their morphological and physiological functions for adapting the crop to the environment (SINCLAIR et al., 2010; GILBERT et al., 2011; LI et al., 2013). Soybean genetic variability enables one to identify cultivars with different growth and physiological characteristics, which can be used to improve yield under adverse climatic conditions. The adaptation to water deficit and high temperatures can be done by evaluating soybean traits in new cultivars in order to improve yield and reduce the yield gap for the current and future climates (BOOTE et al., 2011).

The first step to mitigate yield losses is to identify soybean breeding lines with advantageous traits that can help the crop to adapt to adverse conditions, such as water deficit (LEHMANN et al., 2013). Cultivars characteristics, such as deeper and greater root system (BENJAMIN; NIELSEN, 2006; BORTOLUZZI et al., 2014), soil water conservation (SINCLAIR et al., 2008; GILBERT et al., 2011), nitrogen fixation drought tolerance (SINCLAIR et al., 2007), and less sensitivity of grain filling acceleration under drought (SPECHT et al., 1986; RUÍZ-NOGUEIRA et al., 2001) can be used to develop cultivars adapted to drought.

The time between identification of one of these traits in a soybean breeding line and applying it in a new cultivar is very long, and in some cases, the traits selected may not show a good effect in the field because of climate and soil conditions. One alternative is to test these traits through crop models (SINCLAIR et al., 2010; BOOTE, 2011), evaluating how these traits can affect yield for a specific region. After that, selection of cultivars with desirable traits can be done more effectively because crop models allow simulations of multiple crop seasons, which is an advantage in relation to field experiments (EGLI; CORNELIUS, 2009; WHITE et al, 2011).

Based on what was previously presented, the hypothesis of this study is that through selection of soybean traits specific to tolerance to water deficit, it will be possible to develop better cultivars for both the current and future climates in Southern Brazil improving soybean yield. Therefore, the aims of this study were: (1) to calibrate and test the crop model CSM-CROPGRO-Soybean; (2) to manipulate soybean traits of drought tolerance in the crop model;

(3) to assess soybean yield response and total production for the traits tolerant to drought; and (4) to provide guidelines for genetic breeding programs in order to improve the soybean cultivars in Southern Brazil.

4.2 Materials and Methods

4.2.1 Study region

The region of this study covers most of Southern Brazil and is located between latitudes 20° and 34° South and longitudes 47° and 58° West, corresponding to the soybean breeding zones 1 and 2 (Figure 1 from chapter 2, pg. 29). The Koopen's climate classification of the region includes the following climate types: humid subtropical zone without dry season with hot summer (Cfa) and with temperate summer (Cfb) for most of region, and a smaller area in the north as a tropical zone without dry season (Af), with dry winter (Aw) and with monsoon (Am) (ALVARES et al., 2013). During the soybean growing season, the average air temperature is between 18.7°C and 26.2° C, respectively, for the coolest and hottest (Annex K). In this region, soybean is produced on 11 million hectares and the total production is near to 33 million tons (CONAB, 2015).

4.2.2 Crop Model

The soybean crop model used was CSM-CROPGRO-Soybean, present in the software Decision Support System for Agrotechnology Transfer (DSSAT). DSSAT is a software suite of multiple crop simulator models controlled by different modules responsible for simulating several processes, which interact with each another. The system has the following modules: weather; management (sowing, harvest, irrigation, fertilization, organic matter and others); soil (soils dynamics, temperature, balance of water, carbon and nitrogen); and plant, responsible for simulating crop development and growth (JONES et al., 2003) (Annex C and Appendix D).

The CSM-CROPGRO plant module simulates development and growth of different crops with a common source code, but with different read-in parameter values for different species. In the species file, there are parameters that define tissue compositions, growth and maintenance respiration coefficients, CO₂ response, the base and optimum temperatures for crop development and growth, photosynthesis, and N₂ fixation. For soybean, there are

coefficients in the ecotype file that define common parameters between cultivars within the same maturity groups and that vary less often. The coefficients in the cultivar file vary more often and need to be optimized (initially calibrated from field data) for each cultivar (BOOTE et al., 1998; JONES et al., 2003).

The model has different options for many simulation processes. In the simulations, the reference evapotranspiration was estimated by Penman-Monteith FAO 56 method (ALLEN et al., 1998) and infiltration of water into the soil by soil conservation service method through soil curve number (SOIL CONSERVATIONS SERVICE, 1972). The Ritchie tipping-bucket approach was used for soil water balance (RITCHIE, 1998) and Suleiman-Ritchie approach (SULEIMAN; RITCHIE, 2003) for soil evaporation, while the leaf-level photosynthesis response approach was used to simulate soybean photosynthesis (BOOTE; PICKERING, 1994).

4.2.2 Calibration of crop model

CSM-CROPGRO-Soybean was calibrated using data of crop development and growth from three sites located in southern Brazil: Frederico Westphalen, RS (27°21'38" S; 53°23'48" W; 540 m); Londrina, PR (23°11'34" S; 51°10'59" W; 634 m); and Piracicaba, SP (22°42'14" S; 47°37'30" W; 569 m). Cultivar BRS 284 was used in all places and for assessing the model performance. The cultivar was grown under rainfed and irrigated conditions with three sowing dates in Londrina and Piracicaba, and five sowing dates only under rainfed conditions in Frederico Westphalen, from October to January during 2013/2014 crop season. During 2014/2015 crop season, yield and phenology data were obtained from field experiments at Piracicaba and Frederico Westphalen for testing the calibrated coefficients for the BRS 284 cultivar, evaluating crop model performance with independent observed data, which were not used during calibration process.

For calibration, the first step was to enter all information relative to the experiment, including soil type and characteristics, weather data, sowing date, plant population, row spacing, irrigation and fertilization. After this, calibration process was started by changing genetic coefficients from the initial cultivar coefficients. The procedure followed Hunt and Boote (1998) recommendation, starting calibration of phenological parameters and then growth parameters. The coefficients were calibrated using the generalized likelihood uncertainty method (GLUE) (MAKOWSKI et al., 2002; JONES et al., 2011) as well as based on visual adjustments to observed time-series. The visual adjustments was used due to GLUE

to be a statistical method that considered only end-of-season measurements to estimate genetic coefficients, condition that can lead to incorrect results of in-season measurements.

In addition to cultivar calibration, the soil root growth factor (SRGF) was adjusted based in the root profile observed by Pivetta et al. (2011) for soybean in the same regions of the field experiments. The SRGF is responsible for defining the potential ability of root growth versus the soil profile depth, creating different root profile shape, altering total root water uptake due to root length density. The calibration of the cultivar coefficients was continued till the point that phenological and growth outcomes showed acceptable root mean square error and good linear relationship between measured and simulated values. More details about field experiments and model calibration are shown in chapter 2.

4.2.3 Manipulated soybean traits

In this study, virtual cultivars were developed varying the following soybean traits: deeper root depth in the soil profile; maximum fraction of shoot dry matter diverted to root growth under water deficit; early reduction of transpiration under mild stress; transpiration limited as a function of vapor pressure deficit; N₂ fixation drought tolerance; and reduced acceleration of grain filling period in response to water deficit. The most of these traits were shown to be potential adaptive strategies to increase yield and reduce yield gap associated with water deficit and climate change for soybean (BOOTE et al., 2003; SINCLAIR et al., 2010; BOOTE, 2011).

4.2.3.1 Deeper root depth

Deeper root distribution in the soil profile was evaluated by changing the soil root growth factor in the model, based on two concepts: that a better soil management and genetic modification can improve root growth at depth and increase the water available to the crop, mainly in the layer between 30 and 70 cm (FRANCHINI et al., 2009; BORTOLUZZI et al., 2014). Soil root growth factor determines the potential ability of roots to grow in respective soil layers, altering the shape of root distribution and the potential amount of water that can be extracted by the roots from the soil (MA et al., 2009). In this simulation, total root mass was not changed, rather, the adaptation to drought was based on reducing the root length density in the upper layers and improving it in deeper layers.

The standard soil root growth factor was defined in the calibration process based on the soil characteristics, such as pH and AL^{3+} presence, creating a root profile similar to that observed by Pivetta et al. (2011). In addition, the difference between measured yield and that predicted by the model was minimized. In this step, the measured yields were from IBGE (2015b) for the crop seasons from 1991 to 2013 for the sites in Southern Brazil. The standard soil root growth factor calibrated resulted in an exponential geotropism constant of 3, where the value was used to estimate the soil root growth factor, following equations 1 and 2. After the standard root profile for each site was defined, the new soil profile was created to obtain a better homogenous root distribution versus soil depth than standard values, improving root soil exploration (SINGH et al., 2014). For the deeper root depth trait, the soil root growth factor was estimated using an exponential geotropism constant value of 1.2. In Figure 1 are showed the soil root growth factor values obtained from equations 1 and 2, which were used in the simulations for cultivars adapted and non-adapted to drought:

$$SRGF = \begin{cases} 1 & \text{if } Z \leq 15 \text{ cm} \\ (1 - (Z/Z_{max}))^{WCG} & \text{if } Z > 15 \text{ cm} \end{cases} \quad (1)$$

$$(2)$$

where: SRGF is the soil root growth factor; Z is the depth of layer; Zmax is the maximum depth of the roots (160 cm); and WCG is the exponential geotropism constant that differentiate SRGF shape, being 3 for standard and 1.2 for root shape adapted to drought.

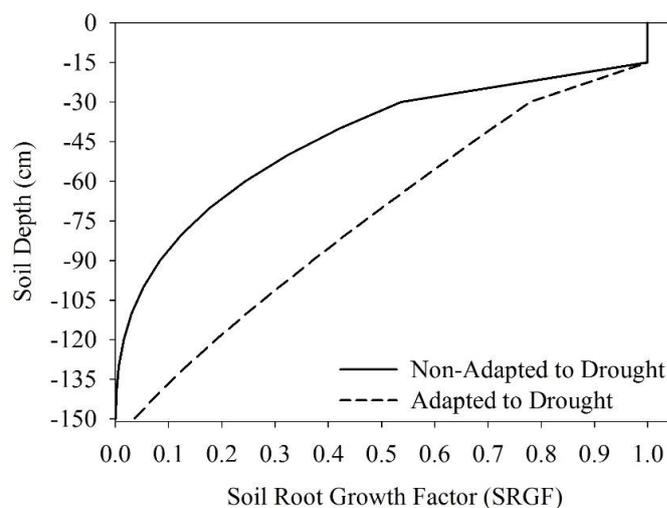


Figure 1 – Soil root growth factor (SRGF) as a function of soil depth for cultivars adapted and non-adapted to drought

4.2.3.2 Maximum fraction of shoot dry matter diverted to root growth under water deficit

The maximum fraction of shoot dry matter diverted to root growth under water deficit is defined in the model by parameter ATOP. If there is no water deficit, then there is no shift in partitioning to roots. The water deficit index (SWFAC) in this model is obtained from the relationship between total root water uptake and potential transpiration. When total root water uptake is less than potential transpiration, the ratio is less than one and water deficits occur, and biomass accumulation is reduced, but the model increasingly allocates assimilates to root mass, consequently, increasing root density and water uptake, but reducing top mass.

The shoot dry matter that is allowed to be diverted to root growth is an important trait for differentiating cultivar adaption to water deficit, as shown by Franchini et al. (2009), who showed that the cultivar EMBRAPA 48 had a better performance under water deficit than BR 16 due to a greater root growth. In the simulations, the standard value adopted was zero, meaning that cultivar has no enhancement of root growth under water deficit, and one, which is a cultivar with a high adaptation to drought, increasingly allocating intended shoot growth biomass to root growth as a function of the SWFAC water deficit signal. Equations 3 and 4 define the fraction of shoot mass diverted to root growth under water deficit:

$$\text{FDTR} = \begin{cases} 0 & \text{if SWFAC} \geq 1 \\ 1 - \text{SWFAC} & \text{if SWFAC} < 1 \end{cases} \quad (3)$$

(4)

where: FDTR is the fraction of dry mass from shoot diverted to root growth under water deficit; and SWFAC is the growth drought stress defined by relationship between total root water uptake and potential transpiration.

4.2.3.3 Early reduction of transpiration under mild stress

The early reduction of transpiration under mild stress was reported in the soybean genotype PI416937 that begins to reduce transpiration early than others, allowing the crop to save water in the soil, and is classified as a potential trait to reduce yield losses under severe water deficits (SINCLAIR et al., 2008). In the crop model, this trait was manipulated using a reduction curve that affects both crop transpiration and photosynthesis as a function of the relationship between total root water uptake (TRWU) and potential transpiration (EOP) (Figure 2). The curve used to adapt the crop to drought simulates an earlier limitation on

transpiration than normal crop response in the standard condition in the model, when the transpiration has a high water demand and/or has a reduction of available water in the soil.

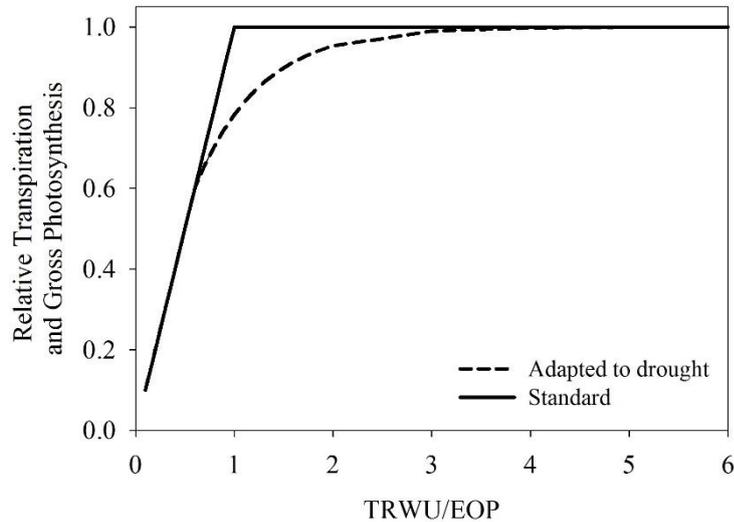


Figure 2 – Relative transpiration and gross photosynthesis estimated for a cultivar adapted and non-adapted to drought (Standard) related with total root water uptake (TRWU) and potential transpiration (EOP)

An earlier cultivar sensitive can be very useful under water stress, because the crop could conserve water and increase its chances of survival. However, it could be a disadvantage under low water stress due to early photosynthesis reduction. Based on this adaptive curve, new values of actual transpiration and gross photosynthesis are estimated through the following equations:

$$EP1 = \text{Min} (EP; ((1.0 - \text{Exp}(-1.527 * \text{TRWU}/\text{EOP}) * EP)) \quad (5)$$

$$A1 = \text{Min} (A; ((1.0 - \text{Exp}(-1.527 * \text{TRWU}/\text{EOP}) * A)) \quad (6)$$

where: EP1 is the new actual transpiration; Min is the minimum value; EP is the original actual transpiration, computed by the model (RITCHIE, 1972; 1985); EOP is the potential transpiration; TRWU is the total root water uptake; A is the original gross photosynthesis, estimated by the model (BOOTE et al., 1998); and A1 is the new gross photosynthesis.

4.2.3.4 Transpiration limited as a function of vapor pressure deficit

The transpiration limited as a function of vapor pressure deficit has the aim to reduce crop transpiration in days when vapor pressure deficit is very high, saving water for use in

later days during the crop cycle. Gilbert et al. (2011) observed different cultivar stomatal conductance response to vapor pressure deficit. According to these authors, the stomatal conductance (and transpiration) of some cultivars responded linearly to vapor pressure deficit, while others had a breaking point that limited stomatal conductance to a lower rate at high vapor pressure deficit, affecting transpiration and photosynthesis rate.

Two soybean genotypes with different stomatal conductance (g_s) were chosen for the analysis, being N01-11136 (insensitive) and PI416937 (sensitive) (Figure 3a). Based on g_s response of these cultivars to vapor pressure deficit, limiting factors for actual transpiration and photosynthesis were obtained for each one of them (Figure 3b). In the model, the first step was to define the stomatal conductance for both genotypes as a function of daily average vapor pressure deficit, following equations 7 and 8 presented in Gilbert et al. (2011). After, a transpiration response ratio between a sensitive and insensitive genotypes was estimated based on the combined stomatal and boundary conductance, following equations 9 and 10. The numerator and denominator of Eq. 10 are similar to photosynthesis versus conductance curves of Gilbert et al. (2011).

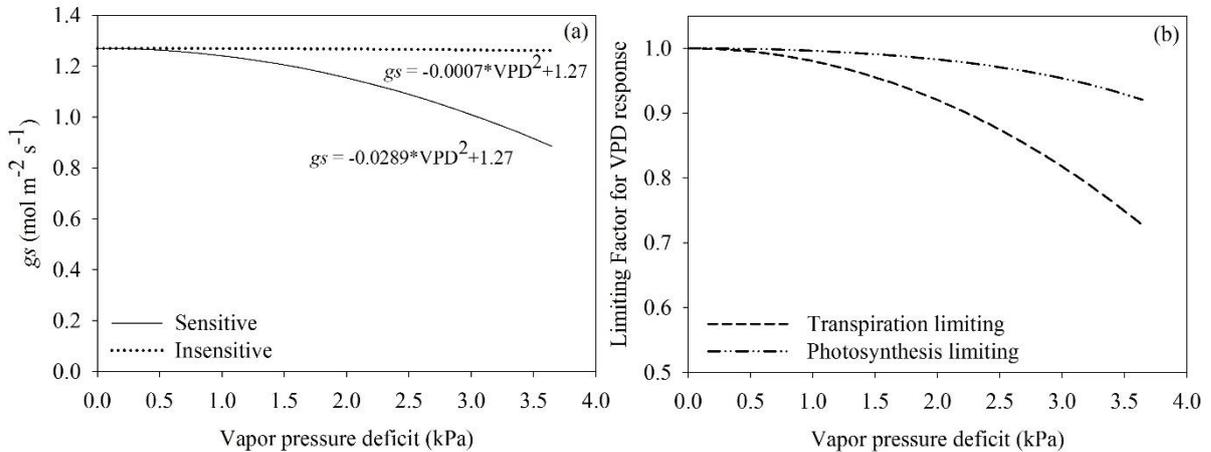


Figure 3 – Stomatal conductance (g_s) for cultivars sensitive and insensitive to VPD response (a) and limiting factor for transpiration and photosynthesis as a functions of average daily VPD (b). Adapted from Gilbert et al. (2011)

$$g_{S_{sen}} = -0.0289 * VPD^2 + 1.27 \quad (7)$$

$$g_{S_{ins}} = -0.0007 * VPD^2 + 1.27 \quad (8)$$

$$Ratio_{EP} = (1/(1/g_{S_{sen}}+1/g_a)) / (1/(1/g_{S_{ins}})+1/g_a) \quad (9)$$

$$Ratio_A = \frac{(38 * (1-\exp(-84 * g_{S_{sen}} - 0.02))/38)+4}{(38 * (1-\exp(-84 * g_{S_{ins}} - 0.02))/38)+4} \quad (10)$$

where: $g_{S_{sen}}$ and $g_{S_{ins}}$ are the stomatal conductance, respectively, for the sensitive and insensitive genotypes, which are function of average daily vapor pressure deficit (VPD). The $Ratio_{EP}$ and $Ratio_A$ are the penalization ratios, respectively, for the actual transpiration (EP) and photosynthesis (A) (Figure 3b), and g_a is the aerodynamic conductance, considered as a constant value of $10 \text{ mol m}^{-2} \text{ s}^{-1}$.

4.2.3.5 Nitrogen fixation drought tolerance

N_2 fixation drought tolerance was manipulated to maintain fixation until lower levels of water availability in the soil, in order to reduce N stress through the improved nitrogen fixation (SINCLAIR et al., 2007). In the crop model, the N_2 fixation drought tolerance was evaluated changing nitrogen fixation parameters that define fixation rate as a function of water deficit index, in this case turgor-based drought stress, in the species file. The turgor-based drought stress is estimated by the relationship between total root water uptake and the potential transpiration multiplied by 1.5, making it a more sensitive index to water deficit than photosynthesis drought stress.

The parameter changed was FNFxD that defines the value of turgor-based drought stress at which N_2 fixation begins to be reduced in linear rate. Two values for the FNFxD, were used, being 0.85 the original value for soybean, and 0.67, which represents a genotype with higher adaptation to drought. The FNFxD of 0.67 was adopted because this value is equivalent to the point at which the photosynthesis drought stress is 1.0, which means that penalization of N_2 fixation occurs at the same time that photosynthesis begins to be penalized by water deficit.

4.2.3.6 Reduced acceleration of grain filling period in response to water deficit

Reduced acceleration of grain filling period in response to water deficit is other important trait to be evaluated. The literature indicates that soybean cultivars typically accelerate maturity and shorten the grain filling phase under advancing water deficit (RUÍZ-NOGUEIRA et al., 2001; SPECHT et al., 2001), which can vary among cultivars (SPECHT et al., 1986). There are parameters in the model that define the degree of sensitivity of the grain filling period to water deficit, in which rate of acceleration to complete the phase can be set, for the period between first seed and maturity. The sensitivity values of 0.0 and 0.7 were used,

respectively for an insensitive cultivar and a sensitive cultivar relative to accelerating the grain filling period in response to water deficit.

4.2.3.7 Combination of traits

The traits evaluated in this study can be included together in only one new cultivar and the yield response may present interactions among them. The yield response may not show linear accumulative results, since the traits can affect each other, but additive yield responses may also occur as reported by Boote et al. (2003, 2011). Thus, yield response for the combination of traits in the model was also evaluated. The association was made between deeper rooting depth, reduced acceleration of grain filling period in response to water deficit and transpiration limitation (early reduction of transpiration and transpiration limited as a function of vapor pressure deficit), creating two different combined traits.

4.2.4 Climate and soil data

The yield responses for the different traits related to drought tolerance were simulated for thirty sites in southern Brazil (Figure 1 from chapter 1, pg. 13). For yield simulation, the inputs in the crop model were current and future climates and soils conditions for these sites. Current climate data were obtained from 1961 to 2014, considering a [CO₂] of 380 ppm. Weather data obtained were maximum and minimum air temperature, rainfall, solar radiation, sunshine hours, wind speed, and minimum relative humidity in daily time-scale from Brazilian Meteorological Service (INMET), Agronomic Institute of Paraná (IAPAR), Brazilian Agricultural Research Company (EMBRAPA) and “Luiz de Queiroz” Agricultural College (ESALQ/USP).

Missing weather data occurred in about 20% of days, a percentage considered acceptable by Grassini et al. (2015). For rainfall, missing data were replaced by data from the closest rainfall station of the Brazilian Water Agency (ANA). Air temperature missing data was replaced by interpolated values when the gaps were no more than three days or estimated from linear relationships between the values from nearby stations, when the gaps were longer, always considering the representativeness of the climate classification between stations (ALVARES et al., 2013) (Figure 1 from chapter 2, pg. 29). Solar radiation, when not recorded, was estimated using sunshine hours or maximum and minimum air temperature when sunshine hours were not available (ALLEN et al., 1998; PEREIRA et al., 2002). Wind

speed missing data were filled out with data from NASA POWER for the period after 1983, while for the previous period, historical average values were used to fill missing data.

Future climate scenarios were created for the same thirty sites, using the baseline of 1961-2014 and the projection for delta mean air temperature. The delta of air temperature between actual and future periods were obtained based on the ECHAM-Eta and HadCM-Eta models with Eta refined model, which generated climate conditions for Brazil based on the A1B scenario (IPCC, 2015). National Institute of Space Research (INPE, 2015) simulated these projections for each quarter (Annex K). HadCN3 was the border condition adopted by INPE, using high model sensitivity for the simulation of weather data. The [CO₂] adopted was 600 ppm for the period of 2041-2070. The rainfall, solar radiation and wind speed were not changed, while relative humidity was recalculated using the projected air temperature, following Tetens' equation (PEREIRA et al., 2002).

Soil profiles were created for each site, identifying the main soil around weather stations. For this, we used the soil map from IBGE (2015a) and the software QGIS 2.6.1. From the soil map was define an area with a radius of 50 km from the weather station. In this analysis was identified the area for each type of soil, where the chosen soil was the one with the largest area around this site. After that, RADAM Project (1974) data were used to get information on sand, clay and silt content, drainage, pH, carbon and nitrogen content for the corresponding type of soil (Annex B).

4.2.5 Yield response and production analysis

For the thirty sites, yield was simulated for the adapted to drought and the standard traits using Nov 15th as the sowing date, which is in the middle of the sowing window of the region, for the current and future climatic conditions. Based on the yield results from these sites for the adapted to drought and standard cultivars, spatial interpolation by ordinary kriging with spherical variogram model was used to create maps with yield for Southern Brazil. The pixel size was 1 km² (100 ha) and the software used was QGIS 2.6.1. The maps were generated to shown the soybean yield for 25, 50 and 75% percentile and the yield response for adapted to drought cultivar in relation to the standard cultivar along Southern Brazil.

Based on estimated yield data, the total soybean production in Southern Brazil was also estimated. The average baseline yield for the region under current and future climates, yield response for single and combined traits, soybean production area density and the area of

each pixel from the map (100 ha) were used to define total production, following equation 11. In the end, the total production was corrected to the residual grain water content of 13%, because the output from the crop model is in a dry matter basis.

$$Tp_j = \sum_{i=1}^n \{(Ay_i + Yr_{ij}) \times PA \times PSA_i\} \quad (11)$$

where: Tp is the total production in the whole area (kg); Ay is the average yield estimated by the model corrected to 13% of grain water content (kg ha⁻¹) for each pixel (i); Yr is the yield response for the trait (j) for each pixel (i) (kg ha⁻¹); PA is the pixel area (100 ha); PSA is the proportion of soybean cultivated area in each pixel (i) (Figure 1 from chapter 1, pg. 13) (ha ha⁻¹); and n is the number of pixels in the region. PSA was obtained by dividing average soybean production area in the pixel, for the period between 2009 and 2013 (IBGE, 2015), by total pixel area (PA).

4.3 Results and Discussion

4.3.1 Crop model performance

The model CSM-CROPGRO-Soybean predicted a mean yield value of 2946 kg ha⁻¹ against observed mean value of 2883 kg ha⁻¹. Linear relationship between measured and simulated yield had “b” value of 1.01 ($R^2 = 0.79$), with a mean and absolute mean errors of 63 and 446 kg ha⁻¹, respectively, which represents 2.2 and 15.6%, and a root mean square error of 550 kg ha⁻¹. There was a good range of yield in these field experiments, from 1172 to 5375 kg ha⁻¹, which improved model evaluation. The crop phases had good agreement between measured and predicted dates of occurrence, resulting in root mean square errors of 3.0, 6.5, 6.2 and 4.5 days, respectively, for the anthesis, first pod, first seed and maturity. Comparing to independent data, the yield and crop phase predicted by the model had again good agreement between values. More details about model performance is describe in chapter 2.

Different authors around the world have observed similar performance for CROPGRO-Soybean to predict yield as observed in this study. The root mean square error (RMSE) was between 201 and 466 kg ha⁻¹ for different cultivars (BAO et al., 2015), sites and crop seasons (BOOTE et al., 2003), using modified adaptation of the model for air

temperature (SAU et al., 1999) and engaging the Asian soybean rust model (RODRIGUES et al., 2013), against 550 kg ha⁻¹ for our study. This model has been tested and adapted for simulated conditions focused on climate change, as response to [CO₂] and air temperature (ALAGARSWAMY et al., 2006; BOOTE et al., 2010; SAU et al., 1999). All these conditions make the model able to simulate soybean yield and management under different climate conditions (JONES et al., 2003; SINGH et al., 2014; BAO et al., 2015).

4.3.2 Baseline and future soybean yield

The simulated soybean yield by CSM-CROPGRO-Soybean ranged from 0 to 5000 kg ha⁻¹ in Southern Brazil (Figure 4). Under current climate conditions, using actual weather data from 1961 to 2014, in the dry years (25%), lower yield occurs in the south of the region (0 - 1400 kg ha⁻¹), with gradual increases from south of Bagé to Iraí (Figure 4a). Around Umuarama and from Ponta Grossa to São Carlos, the yield ranged between 1401 and 2800 kg ha⁻¹ for the dry years. Normal (50%) and wet (75%) years had similar yield patterns as dry years with the most of the region showing two ranges, between 2801 to 4200 kg ha⁻¹ for the normal (Figure 4b), and between 3501 to 5000 kg ha⁻¹ for the wet years (Figure 4c).

When soybean yield was simulated with future climate scenarios, the pattern of yield variation among the regions was similar to current climate, but for the dry years there was an increase of the area with lower yields in the south, while regions with better yields had a larger area caused mainly by [CO₂] increase (Figure 4d). The positive effect of [CO₂] was clear for the normal and wet years (Figure 4e and 4f), where water deficit was lower and soybean crop presented better performance, increasing the area with soybean yield over 3501 kg ha⁻¹.

The soybean yield variability in Southern Brazil is attributed to the rain distribution and soil water availability (FARIAS et al., 2001; BERGAMASCHI et al., 2007). The lower yield observed in the south is associated to low rain and higher sand concentration in the soils on Encruzilhada do Sul, Bagé and Uruguaiana. On the other hand, the higher rain and soil water availability of Cruz Alta improved the yield in the dry years (CUNHA et al., 2001). These simulated yield trends had similar patterns as observed in the data provided by IBGE (2015b) and by the soybean cultivars assessment conducted by Pro-Seeds Foundation (2013), and simulated by Dallacort et al. (2008) with same crop model and by Battisti and Sentelhas (2015), with a simpler model.

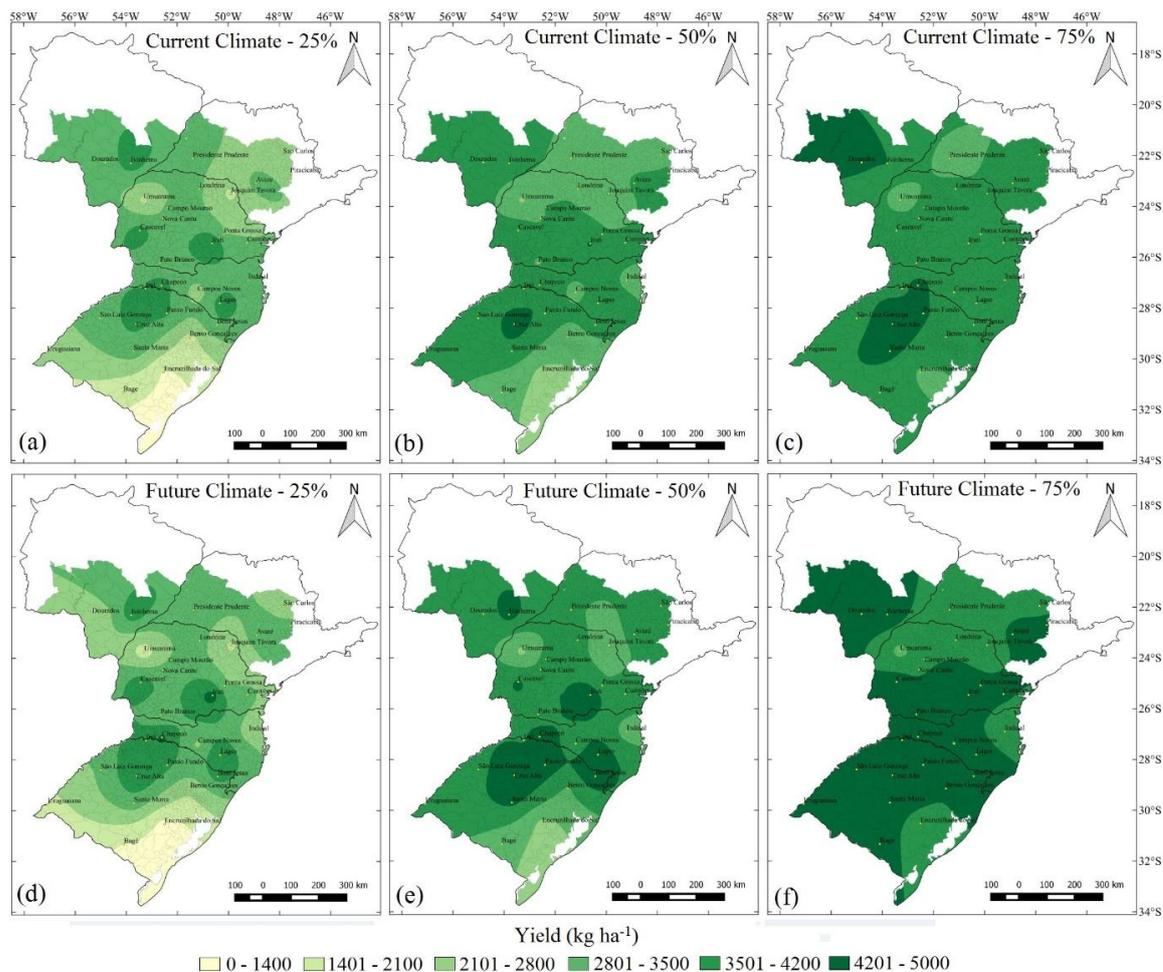


Figure 4 – Soybean yield for the percentile of 25 (a and d), 50 (b and e) and 75 (c and f), simulated by CSM-CROPGRO-Soybean for the current (a, b and c) and future (in the middle of century) (d, e and f) climates in Southern Brazil

The yield simulated for the future climate in the studied region had higher yield than current climate conditions. The first aspect for positive results are associated with the current air temperature and delta air temperature applied to create future climatic scenario. In the region, the current average air temperature during soybean crop cycle was between 18.7°C and 26.2°C, respectively, for Bom Jesus, RS, and Dourados, MS. With the increase in air temperature, caused by climate change, between 2.2 and 4.0 °C, the future air temperature remained in the range considered suitable for soybean, mainly the cooler regions (BOOTE et al., 1998; KUMAGAI; SAMESHIMA, 2014). The second aspect was the positive effect of [CO₂] increase, from 380 ppm to 600 ppm, on the soybean photosynthesis (LEHMANN et al., 2013).

A positive effect of [CO₂] on soybean yield has been observed by many researchers, including Streck and Alberto (2006), who found positive results for rising [CO₂] up to an increase of temperature of 6°C in the same region of this study, while Heinemann et al. (2006)

showed increase in the grain yield with $[CO_2]$ rise at relatively lower temperature in growth chambers. Morgan et al. (2005) observed increase of 15% in soybean yield in the USA, while Hao et al. (2014) observed increase in soybean yield between 26 and 31%. The differences among studies are attributed to the soil, climate and cultivar characteristics, as well as to the future climate scenarios considered.

4.3.3 Yield response for the soybean traits

4.3.3.1 Deeper root depth

Deeper root depth distribution had a positive yield response for the entire region under current (Figure 5a) and for the most of the area for future climate conditions (Figure 5b). Yield gain attributed to this trait was between 1 to more than 300 kg ha^{-1} in both climate conditions, but with future climate showing a greater area with higher yield gains along Pato Branco, Campo Mourão and Joaquim Távora (Figure 5b). The negative response occurred only in a small region at the south of Bagé under future climate, which can be attributed to fewer roots in the upper soil layers to uptake water and nitrogen in the beginning of cycle.

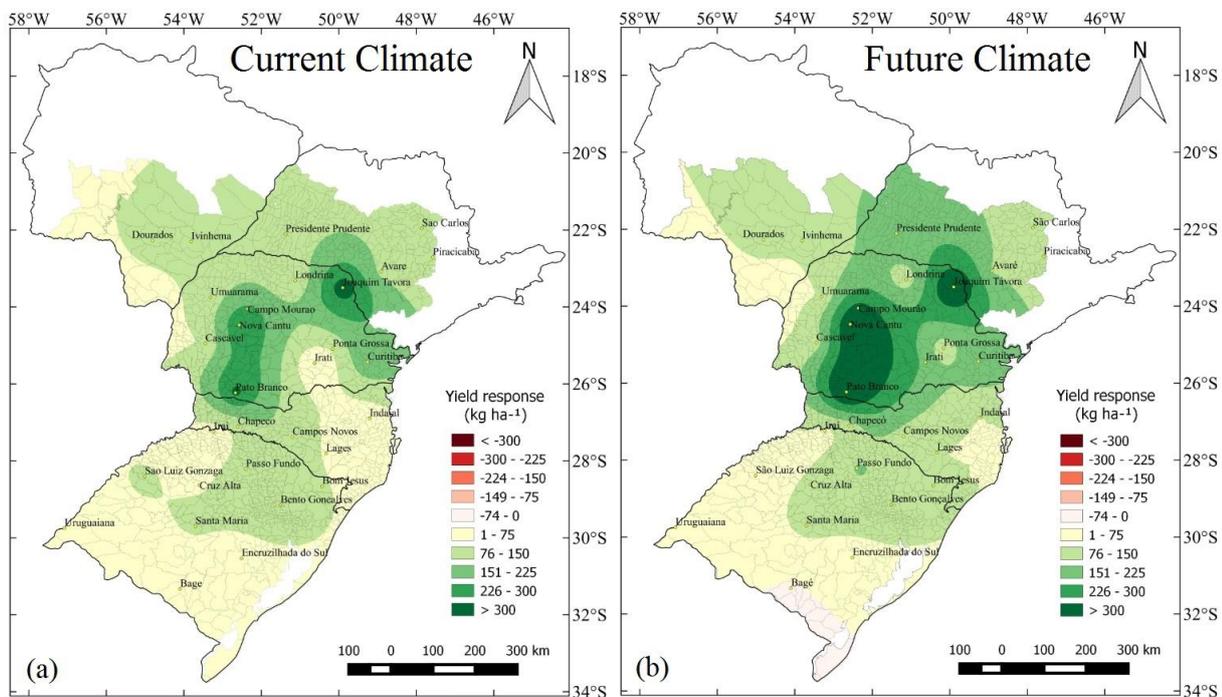


Figure 5 – Soybean yield response using the deeper root depth adapted to drought under current (a) and future (b) climates in Southern Brazil

The yield response is an interaction of conditions for each site (soil and climate) with crop trait, as simulated by Singh et al. (2014), who obtained different interactions between climate condition and traits of chickpea for locations in India and West Africa. In the present study, for example, the area in the south had a similar response for current and future climates (Figure 5), showing that deeper root depth help to reduce water deficit and increase yield in both cases, reaching 150 kg ha^{-1} . In the same region, Bortoluzzi et al. (2014) obtained an increase of 372 kg ha^{-1} in a dry year for soybean when limestone application was used to improve soil chemical conditions and root depth. In the regions of Pato Branco, Campo Mourão and Joaquim Távora, higher yield responses were observed under future than current climate. This means that in addition to the yield increase associated with future climate, yield response was enhanced when water available to the crop was increased with deeper root depth. These findings indicate the importance of cultivar adaptation and crop management for achieving a deeper root depth (FENTA et al., 2014; BORTOLUZZI et al., 2014).

4.3.3.2 Maximum fraction of shoot dry matter diverted to root growth under water deficit

Following the root approach, maximum fraction of shoot dry matter diverted to root growth under water deficit showed a yield response increment of 1 to 75 kg ha^{-1} under current climate for most of the region. In Uruguaiana, Bagé and Encruzilhada do Sul, RS, and near Ivinhema, MS, yield response was negative, between 0 and -74 kg ha^{-1} (Figure 6). Under future climate conditions, increased root mass under water deficit had a similar tendency of yield response as under current climate, but yield was reduced in the south, reaching -149 kg ha^{-1} . On the other hand, the region from Bento Gonçalves to Pato Branco and around Avaré and Joaquim Távora had an expressive yield gain between 151 and 225 kg ha^{-1} under future climate conditions.

The yield response for this trait was dependent on specific site conditions, mainly the total water available to the crop, because when root growth increases, reducing shoot dry mass, the soil should have a good water storage for reducing water deficit and compensating reduction of shoot mass. This compensation occurred at the sites where yield response was positive, but on the other hand, it did not occur in regions with negative response. Similar conditions occur in soils with high bulk density layers, as this condition limits root growth and the crop cannot explore the total water in the soil, making water deficit to occur more often (FRANCHINI et al., 2009).

Hossain et al. (2014) observed that soybean genotypes with greater drought-tolerance were able to improve root mass under drought, a condition that was not observed for a non-drought-tolerant cultivar. In the simulations of the present study, the crop increased root mass under water deficit (Figure 7a), which is a characteristic that helps the crop to explore and use the water in the soil more efficiently. When the soil was better explored, the crop improved the water uptake from the soil (Figure 7b) and thus reduced the water deficit.

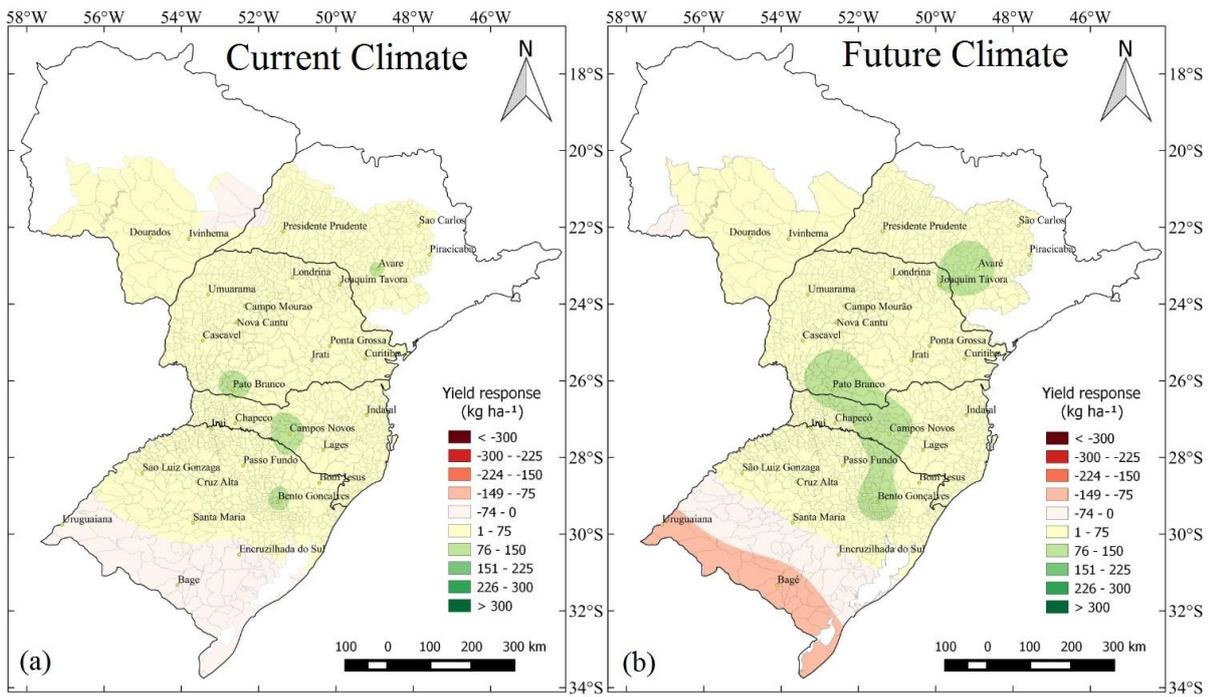


Figure 6 – Yield response for the change of maximum fraction of shoot dry matter diverted to root growth under water deficit (ATOP) under current (a) and future (b) climates in Southern Brazil

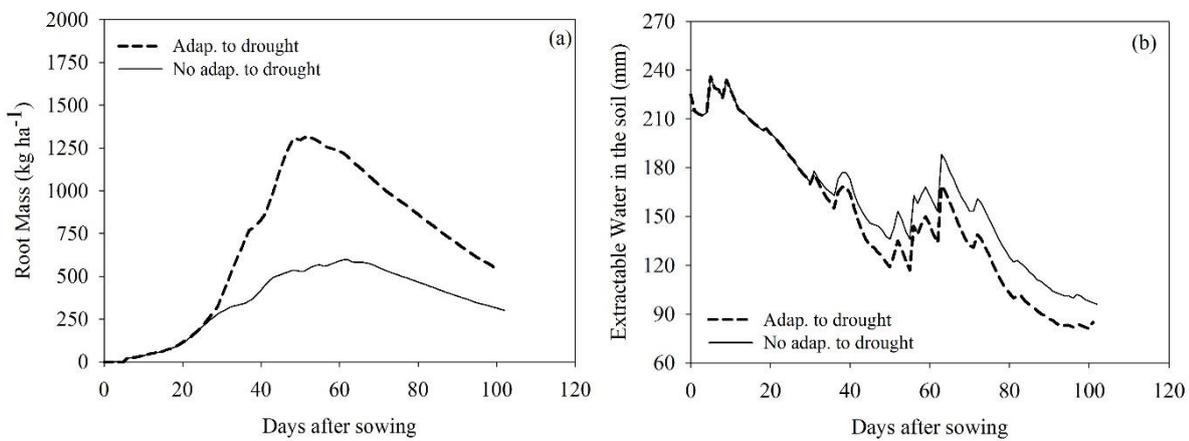


Figure 7 – Root mass (a) and extractable water in the soil (b) for soybean cultivars adapted and non-adapted to drought by maximum fraction of shoot dry matter diverted to root growth under water deficit simulated for a dry year in Piracicaba, SP

4.3.3.3 Early reduction of transpiration under mild stress

This trait is important because it allows the crop to save water early in the cycle to use it in the future when the crop has larger water demand (FARIAS et al., 2001) and greater sensitivity to water deficit during yield formation (DOGAN et al., 2007). Early reduction of transpiration under mild stress had most of the region under current climate showing a negative yield response between 0 and 74 kg ha⁻¹, while the south region, where the water deficit is more frequent, had increases in the yield between 1 and 75 kg ha⁻¹ (Figure 8a). Under future climate, a larger area with positive yield response was observed when compared with current climate conditions (Figure 8a). The best yield response under future climate is because higher air temperature increases water demand and water deficit, making this trait more effective on saving water during the cycle, reducing water stress, which associated with increased [CO₂], enhanced crop yield gains (AINSWORTH and LONG, 2005).

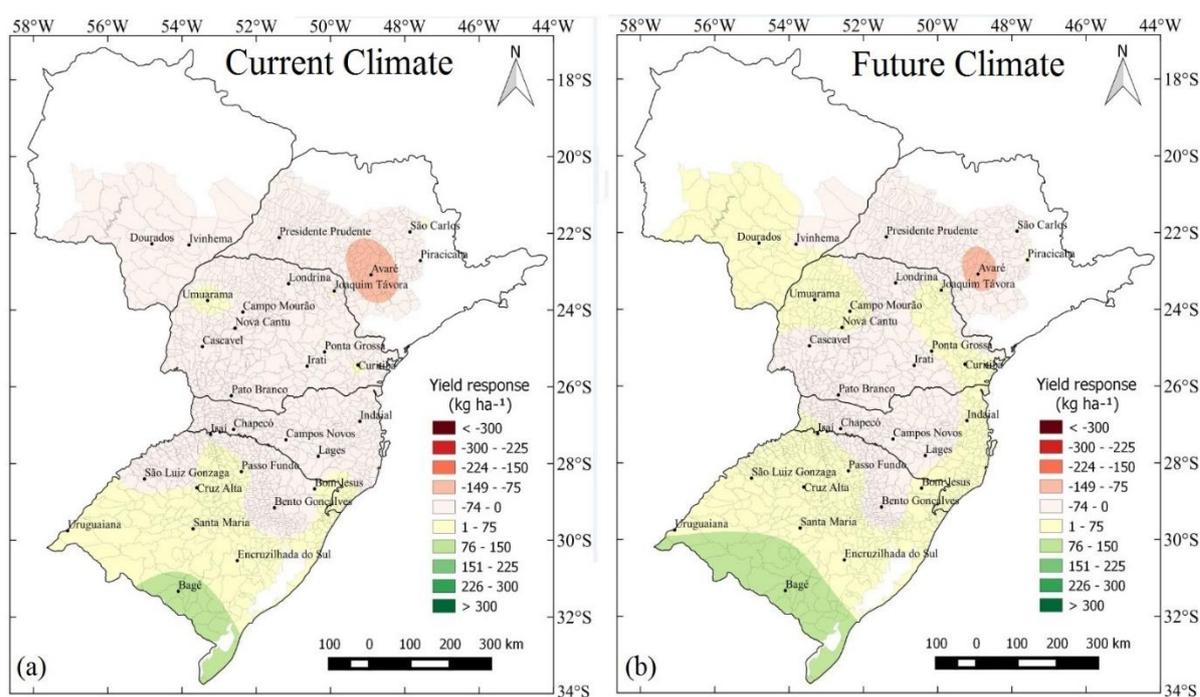


Figure 8 – Soybean yield response using early reduction of transpiration under mild stress, as an adaptation to drought under current (a) and future (b) climates in Southern Brazil

The region had more area showing negative results because the early reduction of transpiration under mild stress also penalized gross photosynthesis at same level as transpiration. This means that when the crop saves water to use later in the cycle, there is a reduction on the photosynthesis early in the cycle, and the water saved early can be not used if

rain conditions improve later in the cycle, causing yield losses. This condition can be observed for a year when water deficit occurred in the first half of cycle in Piracicaba, where the cultivar adapted to drought reduced transpiration, saving water at beginning of the cycle (Figure 9a), and also reducing photosynthesis (Figure 9b). The water saved could be an advantage, but in the second half of cycle, the rainfall was enough for the crop recover the maximum transpiration and photosynthesis, making the early sensitivity of water deficit a disadvantage due to early reduction of the photosynthesis.

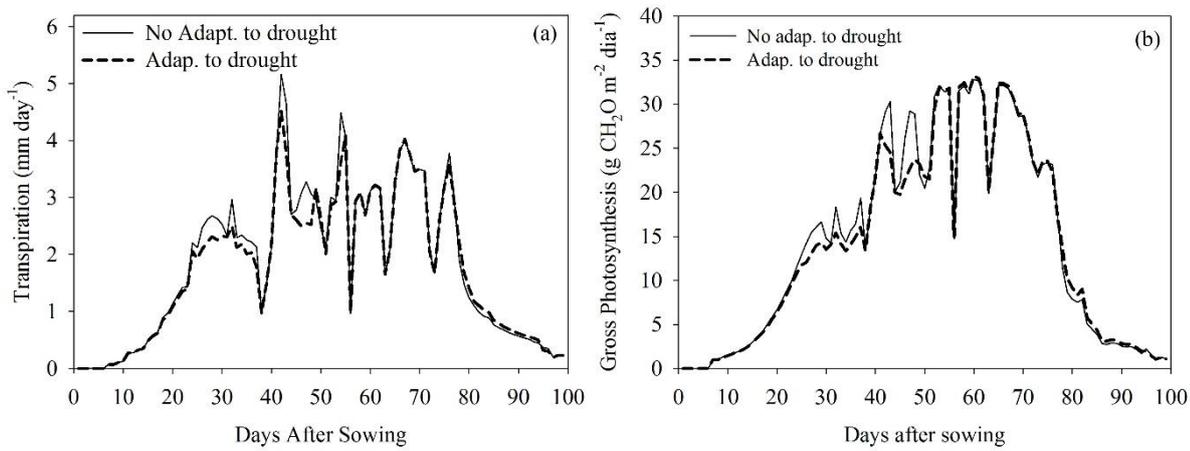


Figure 9 – Transpiration (a) and gross photosynthesis (b) for soybean cultivars adapted and non-adapted to drought by early reduction of transpiration under mild stress, simulated for a year with lower rainfall in the first half of the cycle in Piracicaba, SP, Brazil

It is interesting to illustrate the relationship between the early reduction of transpiration under mild stress with the water available to the crop defined by rainfall and the total available soil water. The yield difference between a cultivar adapted and another non-adapted to drought is dependent on yield level. Bagé, the driest region, had the largest yield response with the trait showing positive gains in most of the years (Figure 10). On the other hand, Cascavel, a region with better rainfall and available soil water conditions had a slight yield response in dry years, but for the most of years showed yield losses (Figure 10).

The interaction between the early sensitivity to water deficit and dry/wet crop seasons was also finding by Sinclair et al. (2010) simulating soybean yield for the USA. These authors observed that yield gain for dry years were close to 700 kg ha⁻¹, whereas in the wet years there was a small yield reduction associated with the reduction in the rate of carbon assimilation. Thus, water saved through early sensitivity to water deficit, even with reduced photosynthesis, is interesting for dry years and in regions that have intense and more frequent droughts as in the southern part of the study region.

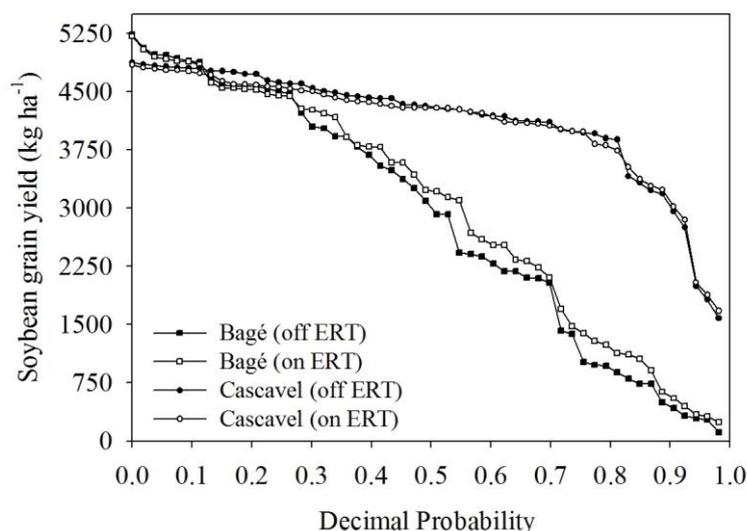


Figure 10 – Soybean yield probability simulated by CSM-CROPGRO-Soybean for future climate using (on) or not (off) early reduction of transpiration (ERT) under mild stress at sites of Bagé, RS, and Cascavel, PR, Brazil

4.3.3.4 Transpiration limited as a function of vapor pressure deficit

While the early reduction of transpiration under mild stress considers both high atmosphere demand and/or low water availability in the soil in the mechanism to reduce transpiration, the option to limit transpiration as a function of vapor pressure deficit uses only the atmospheric water demand, disregarding water in the soil. For this trait, the yield response was positive for most of Southern Brazil (Figure 11). Under current climate, yield gain was between 1 and 75 kg ha⁻¹ in most of region, while the regions between São Luiz Gonzaga, Santa Maria and Encruzilhada do Sul had a greater yield gain, between 75 and 150 kg ha⁻¹, and a small region from Irati to Indaial had reduction between 0 and 74 kg ha⁻¹ (Figure 11a). On the other hand, future climate showed positive yield response for all region, where yield gains were between 1 and 225 kg ha⁻¹ (Figure 11b). Sinclair et al. (2010) simulated a soybean yield gain around of 200 kg ha⁻¹ in the USA, using similar trait approach for the current climate. The difference in the yield response between these studies can be due to climate of the regions and the level of penalization on transpiration and photosynthesis.

The adaptation to drought based in the vapor pressure deficit showed a better yield gain than early reduction of transpiration under mild stress, although both saved water. It happens because this trait had lower penalization on photosynthesis than transpiration. The approach is comparable to that proposed by Gilbert et al. (2011), although in theory the internal CO₂ level (C_i/C_a) would need to be lower than the typical ratio of 0.7 for C-3 plants in order to allow less penalization of photosynthesis than transpiration. Another difference is that

the VPD effect should operate on an hourly step since VPD reaches its maximum value just at mid-day, but the simulations here were restricted by applying the VPD effect on a daily time scale, which is imposed by the restriction of weather data available, and the nature of the evapotranspiration method in the model.

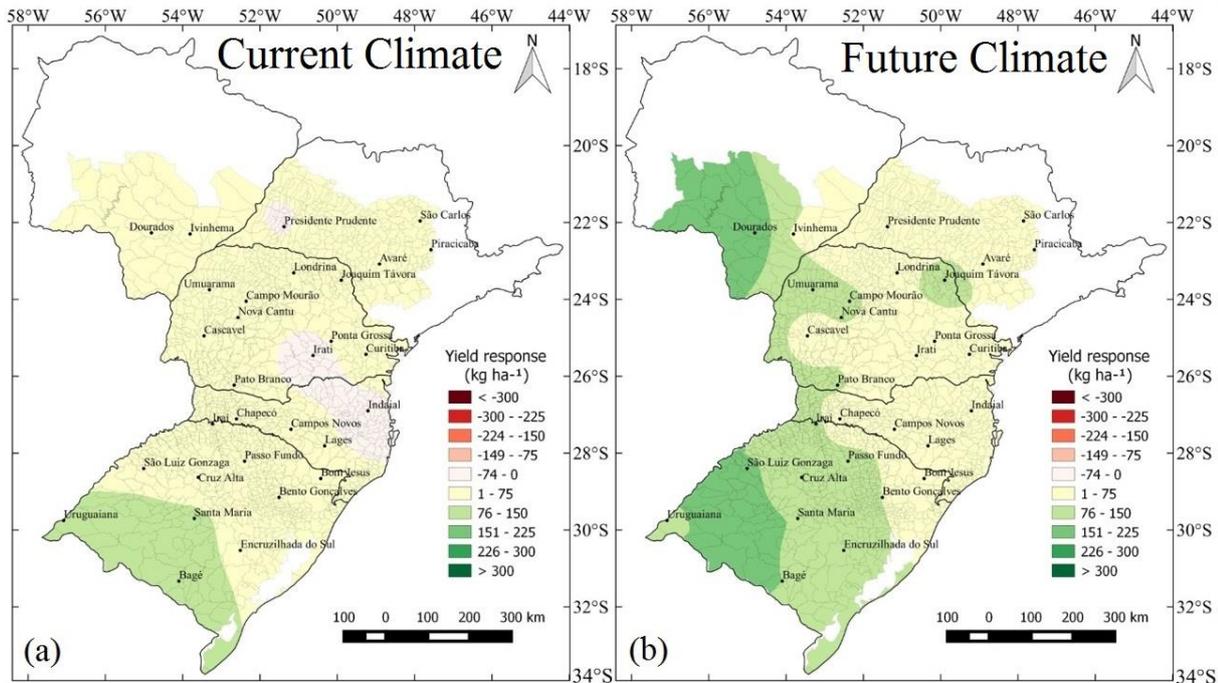


Figure 11 – Soybean yield response for the transpiration limited as a function of vapor pressure deficit, as an adaptation to drought, under current (a) and future (b) climates in Southern Brazil

4.3.3.5 Nitrogen fixation drought tolerance

Nitrogen fixation drought tolerance is associated with a better turgor during soil drying, a condition which supports phloem and xylem flow between leaf and nodules (DEVI; SINCLAIR, 2013). This is an important trait for drought tolerance since most of the nitrogen accumulated by the soybean crop is from biological fixation (SALVAGIOTTI et al., 2008). This trait had a positive outcome for most of Southern Brazil, showing similar yield gain under current and future climate conditions with a yield gain between 1 and 75 kg ha⁻¹ (Figure 12). These values are less than simulated by Sinclair et al. (2010) for the USA, where the yield gains were between 500 and 900 kg ha⁻¹. This difference between these studies is due to the drought tolerance level adopted, with Sinclair et al. (2010) adopting large difference between cultivars. In our study, a smaller difference in drought tolerance was adopted, in part because of CROPGRO model configuration, which considers turgor-based drought stress

(TURFAC) to reduce leaf expansion or N fixation (susceptible lines cannot have their N-fixation more sensitive than is leaf area expansion).

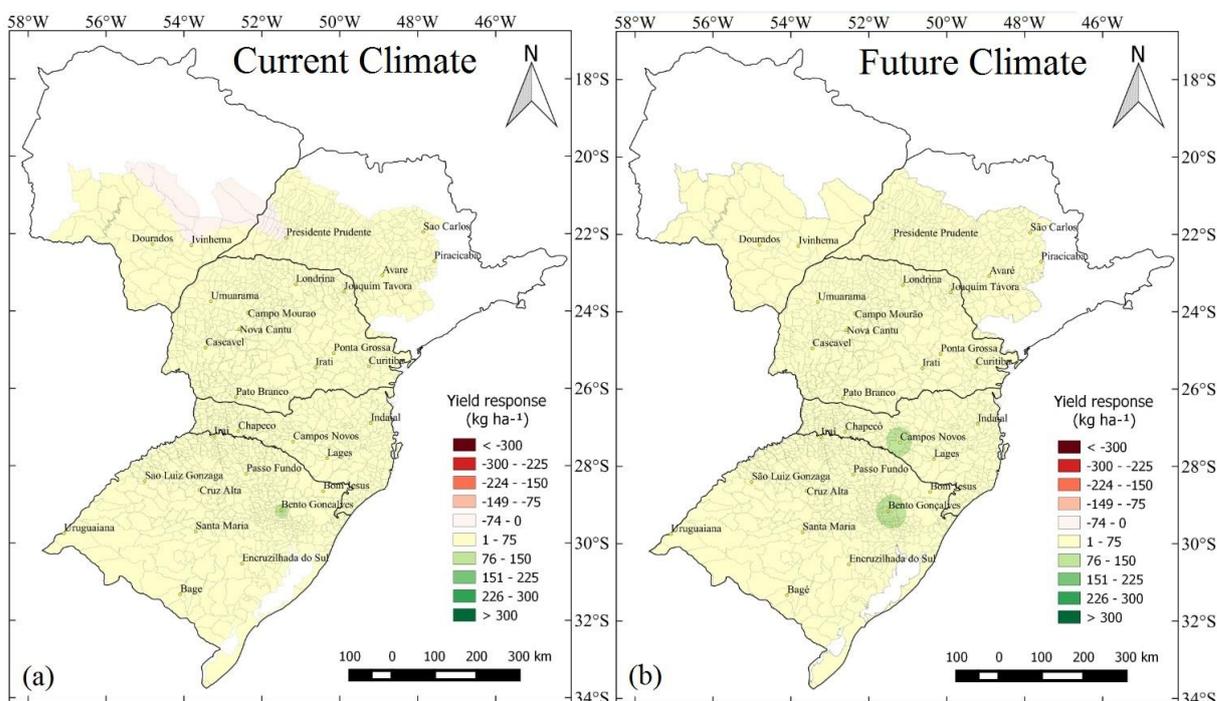


Figure 12 – Yield response using the nitrogen fixation drought tolerance traits for the under current (a) and future (b) climates in Southern Brazil

Under current climate conditions, a small area with negative yield response was found when adopting a cultivar more tolerant to drought, which was attributed to the minor interactions in the model between total grain mass and nitrogen concentration in the seed. These adjustments of grain mass and composition occur as a function of environment, once water deficit effects on photosynthesis reduces grain mass and oil composition, while protein concentration is less affected because of increased nitrogen remobilization (HU et al., 2012).

4.3.3.6 Grain filling period acceleration in response to water deficit

In this trait, the cultivar that not accelerated grain filling period in response to water deficit showed yield gain between 151 and 226 kg ha⁻¹ in the south, but less in the north, where yield gain was between 1 and 75 kg ha⁻¹ for the current climate in the Southern Brazil (Figure 13a). The yield increased in the south due to longer cycle. For example, in Bagé, RS (south), when a cultivar adapted to drought was adopted, the total cycle increased around of 7 days. For this site, the cycle was longer in 58% of crop seasons. For Presidente Prudente, SP

(north), the difference between adapted and non-adapted cultivar was only 2 days for maturity date, altering cycle length in 25% of crop seasons.

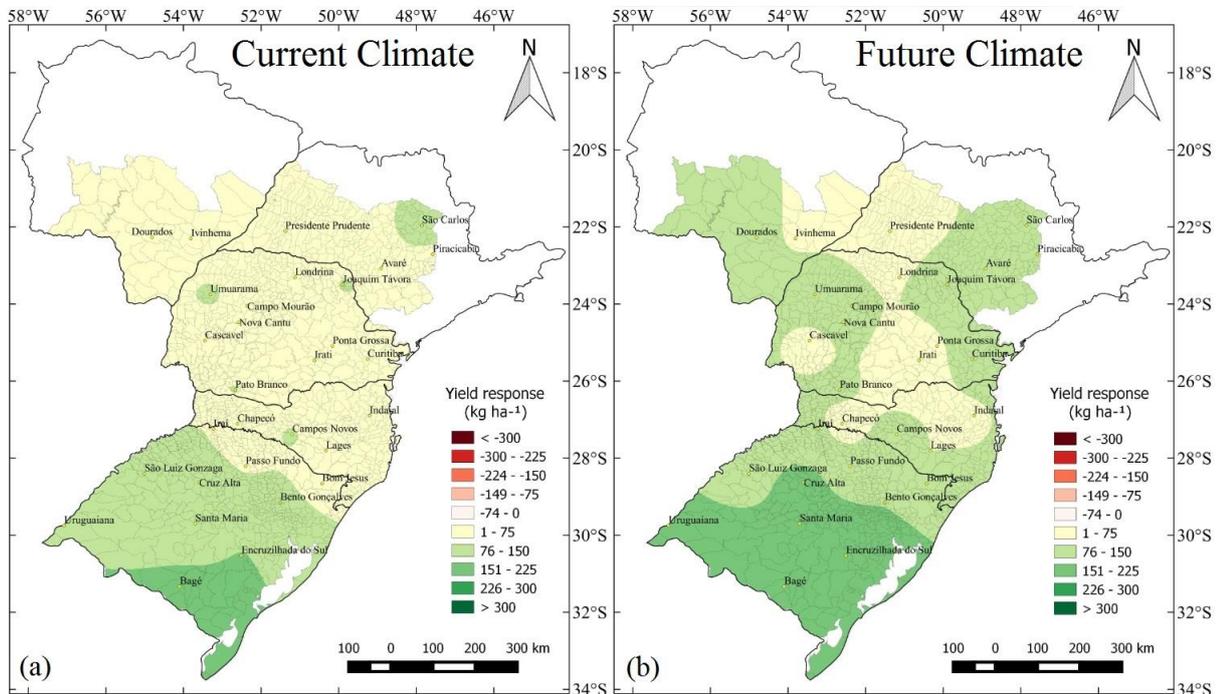


Figure 13 – Soybean yield response for the reduced acceleration of grain filling period in response to water deficit, as an adaptation to drought, under current (a) and future (b) climates in Southern Brazil

Under future climate, the non-accelerated grain filling period in response to water deficit showed a larger area with yield gain between 151 and 226 kg ha⁻¹ for the south, and a range between 76 and 150 kg ha⁻¹ for the northeast and north part of the region (Figure 13b). The crop cycle was shorter under future than current climate. For example, the crop cycle were 124 against 130 days in Bagé, RS, and 100 against 101 days in Presidente Prudente, SP, respectively, for future and current climates. For these two sites, the difference between a cultivar adapted and non-adapted to drought had a similar response of change in the cycle duration for future than current climates.

It may be difficult, in practice, to obtain soybean cultivars that do not accelerate maturity at all under drought stress, but there are different response level between soybean cultivars. Ruíz-Nogueira et al. (2001) reported an acceleration between 6 and 20 days to maturity date for rainfed crop when compared to irrigated soybean. Specht et al. (1986) observed similar difference, between 8 and 12 days, for maturity date as a function of water level for 16 cultivars in two crop seasons.

The effect of the increase on the grain filling period was also evaluated by Boote (2011) in Florida, USA. The author obtained a yield gain of 131 and 151 kg ha⁻¹ under [CO₂] of 350 and 500 ppm, respectively, when grain filling period was increase by 10%, which is similar to the results obtained in the present study. Ruíz-Nogueira et al. (2001) obtained better simulation of maturity date using CROPGRO-Soybean when a coefficient with higher grain filling period acceleration as a function of water deficit was used.

This trait had valuable outcome under water deficit conditions, because when the crop did not accelerate its grain filling period, the crop continued to accumulate photoassimilates, although at lower rate. The lack of sensitivity for grain filling period in response to water deficit can be negative only when the crop dies due to extreme low soil water availability in the end of cycle or when the longer cycle exposes the crop to warmer temperatures (SINGH et al., 2014). In addition to the greater photoassimilation caused by the longer grain filling period, if a rain occurs before the end of crop cycle, yield response can be larger, since crop transpiration and photosynthesis may return to the normal rates, once the photosynthesis apparatus is not affected by the major drought and the crop is able to recover after rewetting. However, the speed of recovery from water deficit is another drought tolerance trait that should be investigated (BRODRIBB, 1996; HOSSAIN et al., 2014).

4.3.3.7 Combination of traits

The traits evaluated in this study can be combined together in a cultivar and apparently do not bring any conflict among them. So if traits are associated and combined, the yield response could be higher (BOOTE, 2011; SINGH et al., 2014). When the traits of deeper root depth and reduced acceleration of grain filling period in response to water deficit with early reduction of transpiration under mild stress (Figure 14a) or with transpiration limited as a function of vapor pressure deficit (Figure 14b) were simulated for the future climate, the yield gain was greater than the single effect of any of these traits. In the both combinations, the yield gain was greater than 150 kg ha⁻¹ for most of Southern Brazil, having great part of the region with yield gain over 300 kg ha⁻¹. When the combinations of traits were simulated for the current climate, the yield gain also increased (results not showed), but in a lower level than future climate, because of the synergistic response between future climate scenario and soybean traits.

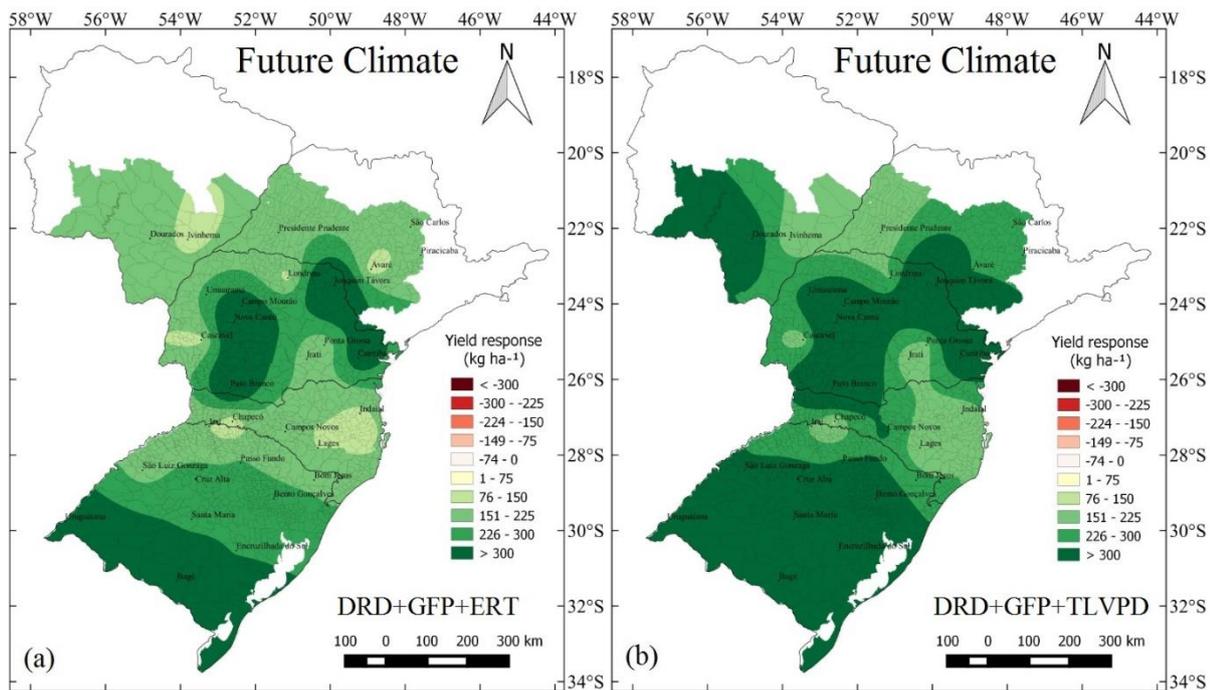


Figure 14 – Soybean yield response for the simulation combining deeper root depth (DRD) and reduced acceleration of grain filling period (GFP) in response to water deficit with early reduction of transpiration (ERT) (a), and with transpiration limited as a function of vapor pressure deficit (TLVPD) (b) under future climate in Southern Brazil

4.3.4 Total soybean production

The baseline yield and the yield traits response were simulated and aggregated for the whole area of Southern Brazil, but it is known that some regions have a greater concentration of soybean production, such as in mid-north of Rio Grande do Sul state, from south-west to northeast of Paraná state and in mid-south of Mato Grosso do Sul state (Figure 1 from chapter 1, pg. 13), and the baseline and traits yield response in these region would have a greater influence on the total production.

The baseline production was 44.50 and 47.41 million tons of soybean for the current and future climate conditions (Table 1). This indicates that the positive effect of CO₂ fertilization under climate change compensated for the losses due to air temperature and transpiration increases, improving production in about 6.5 % by the middle of the century. Bishop et al. (2014) observed through different free air concentration enrichment (FACE) studies that soybean had its yield increased between 2 and 18 %, with average of 10%, when [CO₂] was between 545 and 625 ppm and air temperature between 19.6 and 23.1 °C, similar conditions of the present study.

Table 1 – Soybean grain total production and relative production response for the baseline when using drought tolerant traits under current and future climatic conditions in Southern Brazil

Trait ¹	Current Climate		Future climate	
	Total production ² (Million Tons)	Difference production (%)	Total production ² (Million Tons)	Difference production (%)
Baseline production	44.50	-	47.41	-
DRD	45.98	3.33	49.31	4.00
MFSR	44.85	0.80	47.84	0.91
ERT	44.33	-0.37	47.53	0.25
TLDPV	45.09	1.34	48.83	2.98
NFDT	44.73	0.52	47.70	0.62
GFP	45.36	1.94	48.75	2.82
DRD+GFP+ETL	46.53	4.57	50.53	6.59
DRD+GFP+TLVPD	47.23	6.13	51.66	8.95

¹DRD= deeper root distribution in the soil profile; MFSR= maximum fraction of shoot dry matter diverted to root growth under water deficit; ERT= early reduction of transpiration under mild stress; TLDPD= transpiration limited as a function of vapor pressure deficit; NFDT= N₂ fixation drought tolerance; GFP= reduced acceleration of grain filling period in response to water deficit; ²The production values are expressed for a grain humidity of 13%

In Southern Brazil, the positive soybean yield response is associated with the baseline air temperature and [CO₂] increase. Deryng et al. (2014) showed, through crop simulation model, that when CO₂ fertilization was not considered, most of regions around the world had reduction in soybean yield. On the other hand, CO₂ fertilization associated with higher air temperature increased yield in regions of high latitude, as Argentine, due to lower temperature. Singh et al. (2014) observed that locations with cooler temperature had positive results to chickpea yield when the climate change simulations included increased temperature and [CO₂], opposite of hotter sites, where yield was reduced.

It is important to highlight that the total production predicted using the yield from the crop model does not consider any yield gap from crop management, but if we compare the baseline for the current climate and production observed by IBGE (2015b) and CONAB (2015), which was around of 33 and 37 million tons, respectively, in the crop seasons of 2012/2013 and 2014/2015, the predicted production is reasonable, considering that the yield gap by crop management is around 17 % in Southern Brazil (SENTELHAS et al., 2015).

In relation to the baseline, the production in Southern Brazil increased 3.3 and 4.0 %, respectively, for the current and future climates, when a deeper root depth was considered. Another trait related with root, maximum fraction of shoot mass diverted to root under water deficit showed a positive result on production, but of lower magnitude, corresponding to 0.8 and 0.9 % for the current and future climates (Table 1). Both root traits showed a greater

increase in the production under future than current climates, because these traits improved the water available to the crop, reducing water deficit, and enhancing the positive effect due to CO₂ fertilization (HEINEMANN et al., 2006; HAO et al., 2014).

Early reduction of transpiration under mild stress gave a production response of -0.37 and 0.25 % for the current and future climates, respectively. The second trait related to the transpiration control to conserve water is the limitation of transpiration as a function of vapor pressure deficit, which increased production by 1.3 and 3.0 %, respectively, for the current and future climates (Table 1).

Nitrogen fixation drought tolerance had the positive increase in the production, being of 0.52 and 0.62 %, increasing yield by 0.23 and 0.29 million tons, respectively, for the current and future climates in Southern Brazil. The trait that reduced acceleration of grain filling period in response to water deficit had an increase in the production of 1.9 and 2.8 %, respectively, for the current and future climates, when the cultivar had a grain filling period insensitive to water deficit (not accelerated).

The greatest production of soybean gain was obtained when combined traits were simulated in the crop model, as also observed by Singh et al. (2014), who simulated yield under climate change for chickpea in South Asia and East Africa. In our study, when the simulations were performed using deep root depth (DRD) and reducing acceleration of grain filling period in response to water deficit (GFP) associated with early reduction of transpiration under mild stress (ETL), the results were positive, being greater than the best individual traits response, with production gain of 4.6 and 6.6 %, respectively, for the current and future climates. Following the combined traits, the deep root depth (DRD) and reduced acceleration of grain filling period in response to water deficit (GFP) associated with transpiration limited as a function of vapor pressure deficit (TLVPD) had production gain of 6.1 and 8.9 %, respectively, for the current and future climates (Table 1).

4.3.5 Limiting aspects of this study

The limiting aspects of the present study are highlighted here once they can help to understand the uncertainties of the results and to encourage future researches. The main aspects are:

- Crop model: although the crop model used was tested for different soybean growing conditions in Brazil and around the world, the model cannot represent all interactions present in nature, especially under future climate conditions where crop characteristics may change

due to plant breeding. In the calibration process, the crop model had a mean absolute error of 15%, which can affect the simulated yield, even with a small mean error (2 %);

- Simulation conditions: three aspects about input data deserves to be highlighted: the simulations were made using coefficients for a single cultivar (BRS 284); the sowing date used was only Nov 15th, although this is the main sowing date in the region, sowing earlier or later can change the results due to interactions between the crop and the weather conditions; only the dominant soil of each region was used, which can be a source of variability for the results obtained;

- Climate scenarios: under future climate conditions, only the effect of one scenario (A1B) for the middle of century was used. Another aspect is related to rainfall amount and frequency that were not changed, so the results are limited to the effect of increasing [CO₂] and air temperature;

- Maps generation: the soybean yield and yield response for different traits were evaluated by mapping the results from the thirty sites using interpolation by kriging. So, although this interpolation approach showed good results, different results could be found if other approaches were used;

- Soybean traits: the different approaches and values used for simulated traits were based on the literature. The way that the traits were represented in the model may not be exactly the same as physiological process occur in the field, which can affect yield results. The data used to manipulate the traits in most cases are from specific researches and from soybean lines, which means that these traits can show limiting values until further investigation, including crop and environmental interactions. The deep rooting trait and the N-fixation drought tolerance traits are considered to be conservative compared to what is possible (SINCLAIR et al., 2010; PIVETTA et al., 2011). The shift in partitioning to root during water deficit is a well-accepted and observed phenomenon, but the degree and specific mechanism could differ. The early reduction of transpiration/photosynthesis and the VPD effect on transpiration and photosynthesis, while previously proposed and simulated by Sinclair et al. (2010), remain somewhat uncertain because there is doubt as to the degree to which transpiration can be reduced more than photosynthesis, invoking the requirement for a lower internal leaf CO₂ concentration (lower C_i/C_a ratio) during water deficit. The use of no acceleration of grain filling period in response to water deficit is probably not a conservative trait in retrospect, because most of soybean cultivars accelerate the grain filling period under water deficit although variation exists (SPECHT et al., 1986).

4.4 Conclusions

Through the results obtained in this study is possible to conclude that the CSM-CROPGRO-Soybean was able to predict soybean yield in Southern Brazil and with some manipulation it is possible to create virtual cultivars with adaptation to drought, evaluating yield response to traits for different environmental conditions. The different traits evaluated can help to improve soybean yield under current and future climates in order to develop cultivars with adaptation to drought for Southern Brazil. Following the difference between current and future climates, all traits showed a greater yield gain in the future climate than current climate. The traits of deeper root depth and maximum fraction of shoot dry matter diverted to root growth under water deficit showed positive results for the region, and deeper root depth was the most promising among all traits. From the traits that conserve water to the crop use later in the cycle, consistent positive results were obtained by transpiration limited as a function of vapor pressure deficit, while early reduction of transpiration under mild stress was valuable only for crop seasons or regions where drought is more frequent. Nitrogen fixation drought tolerance and reduced acceleration of grain filling period in response to water deficit showed positive effects on soybean yield in both climate conditions. When deeper root depth and reduced acceleration of grain filling period in response to water deficit were combined with the transpiration limited as a function of vapor pressure deficit or early reduction of transpiration under mild stress, improvement in the yield response were greater than when the traits were evaluated individually. For the breeding programs, traits that create a better root distribution in the soil, greater root mass allocation under water deficit, reduce transpiration with lower penalization in photosynthesis, promote nitrogen fixation drought tolerance, and reduced acceleration of grain filling period in response to water deficit have potential to be included in new cultivars for the Southern Brazil, improving yield and production for both present and future climates.

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5 EVALUATION OF SOYBEAN MANAGEMENT STRATEGIES UNDER CLIMATE CHANGE USING THREE CROP SIMULATION MODELS

Abstract

Strategic crop management can help to improve yield, reduce the yield gap and explore the best combination of inputs available under different environmental conditions. In this way, the aim of this study was to evaluate how the management of irrigation, sowing dates, cultivar maturity groups and planting densities contribute to soybean yields under current and future climates in Southern Brazil. Five sites were selected to represent the range of agroecosystems in Southern Brazil. The evaluation was performed using the crop models DSSAT-CSM-CROPGRO-Soybean, APSIM-Soybean and MONICA. The management options evaluated were irrigation, sowing date, cultivar maturity group and planting density under current climate (1961-2014), and two future projections for the middle century (2041-2070), varying air temperature with high and low sensitivity in the climate model, and assuming a concentration in atmospheric carbon dioxide (CO₂) of 600 ppm. Simulating supplementary irrigation resulted in more stable yields, with a greater increase of yield associated with future than with current climate, however, increasing water demand. Using irrigation, the yield gains were more than 1059 kg ha⁻¹ at Dourados and Avaré using the DSSAT model, and over 502 kg ha⁻¹ in Cruz Alta and Dourados using APSIM and MONICA models, sites that had the greater yield response. For sowing date, the tendencies were mostly similar between climate scenarios, but differing between the models. Using the ensemble of models, yields tend to reduce with sowing date shifting from 15 Sep to 15 Jan, but sowing dates from 15 Sep to 15 Nov produced the most years with above-average yields under all climate conditions. Cultivar maturity group had different responses by model, with APSIM showing that maturity rating of 7.8 was overall the most productive, while DSSAT indicated 7.8 for irrigated conditions and 7.8 and 6.8 for rainfed conditions, and MONICA results were best with 5.8. Analyzing maturity group and sowing date, the uncertainties increase for early and late sowing dates. The plant population between 30 and 50 plants m⁻² were responsible for higher soybean yields in most cases, without any difference between current and future climate. This way, it was possible to observe differences in obtained yield responses as a result of management parameters in the crop models, but in most cases, the models showed that no crop management strategy has a clear tendency to result in better yields in the future. This means that better management for current conditions also represents a viable alternative for the future.

Keywords: Sowing date; Irrigation; Cultivar; Plant density; MONICA; DSSAT; APSIM

5.1 Introduction

The soybean is the main crop grown in Southern Brazil, responsible for 45% of total production in the country (IBGE, 2015), which is one of the largest producers in the world (FAO, 2016). For this crop, there is great economic pressure to improve yield in what are expected to be less favorable climatic conditions in the future (FAO, 2009), namely increasing air temperature and frequency of extreme events (IPCC, 2014), as water deficit that is the

main cause of the soybean yield gap in Brazil (SENTELHAS et al., 2015). White et al. (2011) suggested that cultivars should be adapted to rising CO₂, heat stress and water deficit to prepare for future climate.

The adaptation of soybean to climate change can be achieved through targeted breeding programs, selecting cultivars with higher or more stable yields, for example, through drought tolerance (BENJAMIN; NIELSEN, 2006; SINCLAIR et al., 2008; GILBERT et al., 2011). Another adaptation mechanism is for farmers to decide in favor of management options that have potential to reduce the yield gap, improving crop resilience to climate variations. Among the potential management options, the most feasible are supplementary irrigation (NENDEL et al., 2014; KUSS et al., 2008), variable sowing dates (BAO et al., 2015; RURINDA et al., 2015; DO RIO et al., 2015), maturity group selection (KUMAGAI; SAMESHIMA, 2014), and planting density (KUSS et al., 2008; VAZQUEZ et al., 2014).

Strategic management options need to be evaluated to define the best conditions for soybean growth, analyzing the interactions between crop, the environment and management, increasing the efficiency of production (WHITE et al., 2011). In this context, irrigation can improve the yield by reducing water deficit, especially in soils with less water holding capacity (NENDEL et al., 2014). Irrigation can also show interactions with other management options, such as planting density (KUSS et al., 2008). The available soil water to the crops also interacts with atmospheric CO₂, as observed by Li et al. (2013), with soybean yield increasing with the doubling of current CO₂ only if the soil was well-watered.

Considering adaptive measures required for coping with or exploiting higher air temperatures and increased likelihood of drought stress, Bao et al. (2015) verified that it is possible to avoid soybean heat and drought stresses during the summer by shifting sowing to a later date in Southeastern USA. Regarding crop maturity group, Kumagai and Sameshima (2014) demonstrated that late-maturity cultivars increase yield under climate change in cool regions of Japan, explicitly, due to the post-flowering day-length requirement extending the reproductive period, once the beginning of flowering was accelerated by higher temperatures in late and early-maturity cultivars. On the other hand, Kassie et al. (2015) showed that under current and only wet-scenario future climate does a medium-cycle cultivar has significantly greater yield than a short-cycle maize cultivar, showing that an increased occurrence of water deficit penalizes both of them.

In the process of evaluating potential adaptation pathways, crop models are an important tool that can be used to evaluate different management options based on historical climate conditions and projections for future climate with higher air temperatures and CO₂

(WHITE et al., 2011). One important advantage of crop model is the ability to extrapolate the simulated conditions from a single year or a single experimental site to different sites and climate conditions (JONES et al., 2003). This extrapolation is important because it is not possible to have conclusive results stemming from variable crop management based only on one field experiment (EGLI; CORNELIUS, 2009).

Crop models have been test widely in studies on crop management, as with irrigation (DOGAN et al., 2007), cultivars and maturity groups (BOOTE et al., 2003; BAO et al., 2015), sowing dates (DALLACORT et al., 2008), planting density (KEATING et al., 1988), different environments (ASSENG et al., 2013) and climate change conditions (ALAGARSWAMY et al., 2006; NENDEL, 2009). However, crop models are wrought with inherent uncertainties (BASSU et al., 2014; LI et al., 2015; MARTRE et al., 2015), which can be reduced using multi-model simulation ensembles (RÖTTER et al., 2012; ASSENG et al., 2013).

Based on this, the aim of this study was to evaluate how the crop management options of irrigation, sowing dates, cultivars maturity group and planting densities can contribute for increasing the resilience of soybean cropping under future climate conditions with increased air temperature and [CO₂], compared to the current climate. Resilience in this case is measured by the distribution of grain yields, simulated by three crop models for five sites in Southern Brazil.

5.2 Material and Methods

5.2.1 Sites, climate and soil data

The sites selected for simulations were in the respective municipalities and states of Cruz Alta, RS (28°37'48" S; 53°36'00" W; 472 m ASL), Ponta Grossa, PR (25°05'24" S; 50°09'36" W; 969 m ASL), Campo Mourão, PR (24°04'58" S; 52°21'36" W; 616 m ASL), Avaré, SP (23°04'48" S; 48°54'36" W; 813 m ASL), and Dourados, MS (22°16'12" S; 54°48'36" W; 408 m ASL). These five sites were selected to represent a total of thirty that define a range of soil and climate conditions in Southern Brazil (Figure 1 from chapter 1, pg. 13; Figure 1 from chapter 2, pg. 29; Annex K), following the stratified sampling method recommended by van Bussel et al. (2016). The reduction from thirty to five was based on a climate cluster analysis of the Ward method, using an index of Euclidean distance in the software Action 2.9. The analysis matrix contains the thirty sites in the line and in the columns the average of minimum and maximum air temperature, and total and standard

deviation of rainfall during the soybean growing season. The location of the five sites in Brazil, together with a diagram of the final divisions in the cluster analysis, is presented in Annex J.

The simulations were performed using a baseline and two future climate conditions. The baseline climate data were obtained for the period from 1961 to 2014, totaling 53 crop seasons, including maximum and minimum air temperature, rainfall, solar radiation, wind speed and relative humidity. The climate data were obtained from the Brazilian Meteorological Service (INMET), Agronomic Institute of Paraná (IAPAR), Brazilian Agricultural Research Company (EMBRAPA), and Brazilian Water Agency (ANA). The baseline climate assumes constant atmospheric CO₂ at the current 380 ppm (NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION'S / EARTH SYSTEM RESEARCH LABORATORY - NOAA/ESRL, 2015).

The baseline data were used to create the future climate scenarios with a delta projection for the difference between the future and baseline daily mean air temperature. The delta of air temperature was obtained from National Institute of Space Research (INPE, 2015), which used the climate models ECHAM-Eta, HadCM-Eta and Eta-refined to simulated the future projections, using the climate model HadCN3 as the border condition for Brazil. The two projections for the future, low and high, differ due to climate model sensitivity parameters used in the simulation based on the A1B scenario (IPCC, 2007). The deltas of air temperature used for each quarter are showed in Table 1.

Table 1 – Delta of air temperature by quarter and different sensitivity scenarios within A1B simulated by the National Institute of Space Research (INPE, 2015) for different sites mid-century (2041-2070)

Sites	Delta for air temperature								CO ₂	
	DJF ¹	MAM	JJA	SON	DJF	MAM	JJA	SON	ppm	
	Low (°C)				High (°C)				Current	Future
Avaré	2.0	2.0	2.4	2.8	3.2	3.0	3.2	3.8		
Campo Mourão	2.0	2.0	2.2	2.6	3.2	3.2	3.4	3.6		
Cruz Alta	1.6	1.8	1.8	2.0	2.4	2.4	3.2	2.6	380	600
Dourados	2.4	2.6	2.4	3.0	3.6	3.8	3.6	4.0		
Ponta Grossa	2.0	2.0	2.2	2.4	2.8	2.8	3.2	3.4		

¹DJF= December, January and February (summer); MAM= March, April and May (fall); JJA= June, July and August (winter); SON= September, October and November (spring)

The delta of air temperature was applied at the same level to maximum and minimum air temperatures, while ambient CO₂ of 600 ppm was considered for both future scenarios,

being the reference projection for the year 2055 (IPCC, 2014). The rainfall was not changed because the climate models do not show a clear rainfall tendency in the assessed regions (MARENGO et al., 2010), and the downscaling showed bias for the spatial and temporal patterns of rainfall (CARBONE et al., 2003). Solar radiation and wind speed were not changed, while relative humidity was recalculated using the new air temperature, but with the same absolute humidity, following Tetens equation (ALLEN et al., 1998).

The main soil type of each site was defined using the soil map from the IBGE (2014), from where it was defined two soil types, oxisols and acrisols (Annex B). After defining the main soil type of each site, the silt, clay and sand content and characteristics of drainage, pH, carbon and nitrogen content in the soil were defined based on the soil data from RADAMBRASIL (1974). With these data, the saturation, field capacity and permanent wilting point of each soil were determined through pedotransfer functions developed by Reichert et al. (2009). The data shown in Annex B were used to build the soil profiles for APSIM and DSSAT crop models, limiting soil depth to 150 cm, while in the MONICA model the soil hydraulic properties were defined by selecting a texture class with similar properties from model default parameters, which in this case was a loamy clay (“T1”). Since this default setting assumes a non-structured soil with very low drainage, the drainage coefficient in MONICA was set to 1.0 to mimic the fast-draining behavior of the sand-sized pseudo-aggregates predominant in Brazilian Oxisols and Acrisols.

5.2.2 Crop Models

Three crop models were used for simulations: Crop Simulation Model – CROPGRO – Soybean, present in the software Decision Support System for Agrotechnology Transfer (BOOTE et al., 1998, 2003; JONES et al., 2003) referred to as DSSAT; the Agricultural Production Systems Simulator (ROBERTSON and CARBERRY, 1998; KEATING et al., 2003) referred to as APSIM; and the Model for Nitrogen and Carbon in Agroecosystems (NENDEL et al., 2011) referred to as MONICA. See Annex C and Appendix D for more details about crop models.

The crop models were calibrated using observed results of intermittent growth (leaf area index, leaf, stem and pod dry mass, plant width and height) sampled six times along the crop cycle, variables obtained in the harvest (yield, harvest index, grain weight, grain and pod number) and timing of crop development (flowering, 1st pod, 1st seed and maturity). The data was collected during the 2013/2014 crop season in Frederico Westphalen, RS (27°21’38” S;

53°23'48" W; 540 m ASL) under rainfed conditions; Londrina, PR (23°11'34" S; 51°10'59" W; 634 m ASL) under rainfed and irrigated conditions; and Piracicaba, SP (22°42'14" S; 47°37'30" W; 569 m ASL) under rainfed and irrigated conditions. Five sowing dates were chosen at Frederico Westphalen and three at both Londrina and Piracicaba, between October and January, totaling 17 field experimental variations.

The cultivar used in all experiments was BRS 284, with maturity group 6.5, an indeterminate growth habit, and a conventional material. In the field experiments fertilizer was applied to sustain crop growth without nutrient deficiency and was performed according to soil analysis, applying mainly phosphorus and potassium and using rhizobium inoculation to improve soybean nitrogen (N) fixation. The spacing between rows was between 0.45 and 0.50 m, with the plant population between 26 and 32 plants m⁻². Piracicaba had full irrigation, while in Londrina irrigation was gauged to supply an estimated 75% of potential evapotranspiration.

5.2.3 Crop Management

5.2.3.1 Water Management

Variations in water management were evaluated with respect to yield response to supplementary irrigation compared to rainfall-limited conditions. Under rainfed conditions, rainfall records from each site were used, and these data were not changed for the simulated future climate. Under irrigated management, automatic irrigation was used in each crop model, so that simulated irrigation was applied when plant-available water in the soil dropped below 70%. This percentage of plant-available water is computed as the ratio of immediate water content minus water content at the permanent wilting point, divided by the difference between the field capacity and the permanent wilting point, which was computed for the immediate rooting depth down to a maximum depth of 60 cm (ALLEN et al., 1998). The irrigation amount applied was 8 mm day⁻¹ from sowing until soybean maturity, this value is based on the common sprinkler systems implemented in Brazil, considering an irrigation efficiency of 100%.

5.2.3.2 Sowing date

The preferential sowing date for Southern Brazil is mid-November (FIETZ; RANGEL, 2008; DO RIO et al., 2015), to obtain the highest yield. Currently, the majority of

farmers are sowing soybeans earlier to enable two crop seasons in the same agricultural year, with maize or another soybean crop in the off-season. Based on this sowing date tendency, five sowing dates, namely 15 Sep, 15 Oct, 15 Nov, 15 Dec and 15 Jan were evaluated at each site for the three climate scenarios.

5.2.3.3 Maturity group

In Southern Brazil soybean maturity groups from 5 to 8 are cultivated (ALLIPRANDINI et al., 2009), creating different crop cycle durations from sowing to maturity. Based on this information and the most frequently selected maturity group from soybean cultivar competitions (PRO-SEEDS FOUNDATION, 2013), three maturity groups (MG) were chosen to use in this simulation: 5.8; 6.8; and 7.8. The coefficients obtained for each crop model were from the cultivar BRS 284, MG 6.5. Based on this cultivar, the coefficients related to crop development were adapted to obtain the maturity groups proposed. According to Kaster and Farias (2012), each tenth (0.1) of change in MG, equates to a difference between 1.5 and 2 days for cultivar maturity. Based on this, using photoperiod sensitivity from the default settings for each MG, the photothermal time was proportionally changed in each crop phase to obtain the difference in number days to maturity in relation to BRS 284. The differences were -11, +5 and +20 days, respectively, for MG 5.8, 6.8 and 7.8.

5.2.3.4 Plant Density

The plant densities adopted were 10, 30 and 50 plants m^{-2} , which can be considered, respectively, low, normal and high population in relation to the recommendations by EMBRAPA (2013) for the region. Plant density simulations were performed for the crop models APSIM and DSSAT. For MONICA crop model, there is no response to this management option, so that this variation is not included in the simulations.

5.2.4 Statistical Analysis

Grain yield was the output used to evaluate each soybean management decision. The first step was an analysis of variance (ANOVA), to identify possible interactions between the factors (level), which were: three climate scenarios; five sites; two water management options; five sowing dates; three maturity groups; and three plant densities. The ANOVA was

performed independently on each crop model results set, where each combination of factors had 53 repetitions (crop seasons). After defining the interactions between the factors, a comparison of means was performed via a Tukey test of 5% probability and/or analyzing the results by graphical comparison. In the graphical comparison were used the mean yield simulated by crop model in each climate scenario and site, while the relative soybean yield was obtained dividing the result from each crop season by the mean of each set from crop model, climate scenario and site.

5.3 Results and Discussions

5.3.1 Crop model performance

The crop models need to be able to simulate yield in different environmental conditions. The models DSSAT and APSIM showed a slight tendency toward overestimation of yield, respectively, of 3.1 and 2.8%. MONICA, however, showed under-prediction of 1.6%. Despite this difference between measured and simulated yields, the models replicated the yield tendency, in that under dry, normal and wet conditions, the models captured the environmental effects on yield (PIRTTIOJA et al., 2015). The dates of occurrence of crop phases were well estimated by all three crop models, especially the timing of beginning of flowering (R1) and maturity (R7), partly due to these phases being better defined, in all models, than beginning of pod formation (R3) and beginning of grain filling (R5). See chapter 2 for more details about crop models performance.

5.3.2 Crop managements and their interactions

Based on the statistical analysis and the aim to evaluate management to improve soybean resilience by climate scenario and site, a total of six interactions were selected to describe the results for each management option. These interactions were: (1) scenario, site and water management; (2) scenario, site, water management and sowing date; (3) scenario, site, sowing date and maturity group; (4) scenario, water management and maturity group; (5) scenario, site and plant density; and (6) scenario, sowing date and plant density (Table 2). Although in some cases one or more models did not show statistically significant variation due to these factors, the results were reported if at least one model had statistically significant results at a level of $p < 0.05$.

Table 2 – *p* value for the analysis of variance (ANOVA) obtained by general linear models (GLM) for soybean grain yield in function of scenarios, sites, water management (WM), sowing date (SD), maturity group (MG), plant density (PD) and their interactions for each crop models

Effects	DF ²	Crop Models		
		APSIM	DSSAT	MONICA
Scenarios	2	<0.001	<0.001	<0.001
Sites	4	<0.001	<0.001	<0.001
WM	1	<0.001	<0.001	<0.001
SD	4	<0.001	<0.001	<0.001
MG	2	<0.001	<0.001	<0.001
PD	2	<0.001	<0.001	-. ³
Scenarios*Sites	8	<0.001	<0.001	<0.001
Scenarios*WM	2	<0.001	<0.001	0.605
Scenarios*SD	8	<0.001	<0.001	<0.001
Scenarios*MG	4	<0.001	<0.001	0.034
Scenarios*PD	4	0.031	<0.001	-
Scenarios*Sites*WM ¹	8	0.000	0.004	0.795
Scenarios*Sites*SD	32	<0.001	<0.001	<0.001
Scenarios*Sites*MG	16	<0.001	<0.001	0.950
Scenarios*Sites*PD ¹	16	0.818	0.023	-
Scenarios*WM*SD	8	<0.001	0.375	0.599
Scenarios*WM*MG ¹	4	<0.001	0.048	0.999
Scenarios*WM*PD	4	0.268	0.617	-
Scenarios*SD*MG	16	<0.001	<0.001	<0.001
Scenarios*SD*PD ¹	16	0.001	<0.001	-
Scenarios*MG*PD	8	0.469	0.987	-
Scenarios*Sites*WM*SD ¹	32	0.953	<0.001	1.000
Scenarios*Sites*WM*MG	16	0.839	1.000	1.000
Scenarios*Sites*WM*PD	16	1.000	1.000	-
Scenarios*Sites*SD*MG ¹	64	<0.001	0.216	<0.001
Scenarios*Sites*SD*PD	64	1.000	1.000	-
Scenarios*Sites*MG*PD	32	1.000	1.000	-
Scenarios*WM*SD*MG	16	0.214	0.516	1.000
Scenarios*WM*SD*PD	16	1.000	0.987	-
Scenarios*WM*MG*PD	8	1.000	0.907	-
Scenarios*SD*MG*PD	32	0.999	1.000	-
Scenarios*Sites*WM*SD*MG	64	1.000	1.000	1.000
Scenarios*Sites*WM*SD*PD	64	1.000	1.000	-
Scenarios*Sites*WM*MG*PD	32	1.000	1.000	-
Scenarios*Sites*SD*MG*PD	128	1.000	1.000	-
Scenarios*WM*SD*MG*PD	32	1.000	1.000	-
Scenarios*Sites*WM*SD*MG*PD	128	1.000	1.000	-

¹Interaction considered for the results analysis of soybean yield; ²DF= degrees of freedom; ³Factor plant density was not simulated by MONICA model

5.3.2.1 Water Management

The use of supplementary irrigation showed interactions between scenarios and sites. For all sites and scenarios, the crop models DSSAT and MONICA showed statistically significant differences between irrigated and rainfed conditions, while APSIM did not show any significant difference for the sites of Ponta Grossa and Campo Mourão under current conditions, and Ponta Grossa for the low and high climate sensitivity future scenarios (Figure 1). These results are associated with lower air temperatures in Ponta Grossa, which had the lowest water requirement and less water deficit for all climate scenarios. For Campo Mourão, the better soil and climatic conditions obviated any positive results of irrigation for current climate, but with an increase of air temperature in the future, the supplementary irrigation resulted in improvement of soybean yields. Nendel et al. (2014) also observed that yield response is higher under future scenarios than under current conditions using irrigation.

The APSIM model was less sensitive to water deficit, with yields reaching a maximum of 6340 and 5182 kg ha⁻¹, respectively, for irrigated and rainfed conditions that occurred for the low climatic sensitivity scenario in Cruz Alta (Figure 1b). The models more sensitive to water deficit were DSSAT, with intermediate results (Figure 1d, 1e and 1f), and MONICA, which had lower mean yields (Figure 2g, 2h and 2i). Relative yield gains when used irrigation, considering all sites, were of 9, 12 and 13% for APSIM, 29, 35 and 40% for DSSAT, and 11, 11 and 11% for MONICA, respectively for baseline, low and high future scenarios.

The highest yield gains using supplementary irrigation simulated with the DSSAT model were at Dourados and Avaré, with gains over 1059 kg ha⁻¹, and in Dourados and Cruz Alta, when yield was simulated with APSIM and MONICA, with values over 502 kg ha⁻¹ (data not shown). In Ponta Grossa and Campo Mourão, the yield gain was lower than the other sites for all crop models, with yield gains no more than 1058 kg ha⁻¹. Interesting is that the yield gains simulated by APSIM and DSSAT increased in both future climate scenarios, when compared with current conditions, although the simulations also indicated an increase in the amount of irrigation required (data not shown). The MONICA model, however, had nearly constant yield gain, amount of irrigation and number of irrigation applications across climate scenarios and sites.

Supplemental irrigation showed potential as a way to improve the yields in both current and future climatic conditions, where most crop models have shown that yield gains can be higher in the future, as associated with more plant-optimal water conditions and yield

gains of soybean due to CO₂ rise (LI et al., 2013). Another point that needs to be explored is the use of conservation practices to reduce crop water demand. Devkota et al. (2015) observed that conservation agriculture practices, in this case for rice-wheat systems, reduced the water requirement three-fold when compared with conventional management. In this context, it is possible to consider irrigation only being applied during the crop phases in which the crop is most sensitive, reducing the water requirement without drastically reducing yield for soybeans (DOGAN et al., 2007).

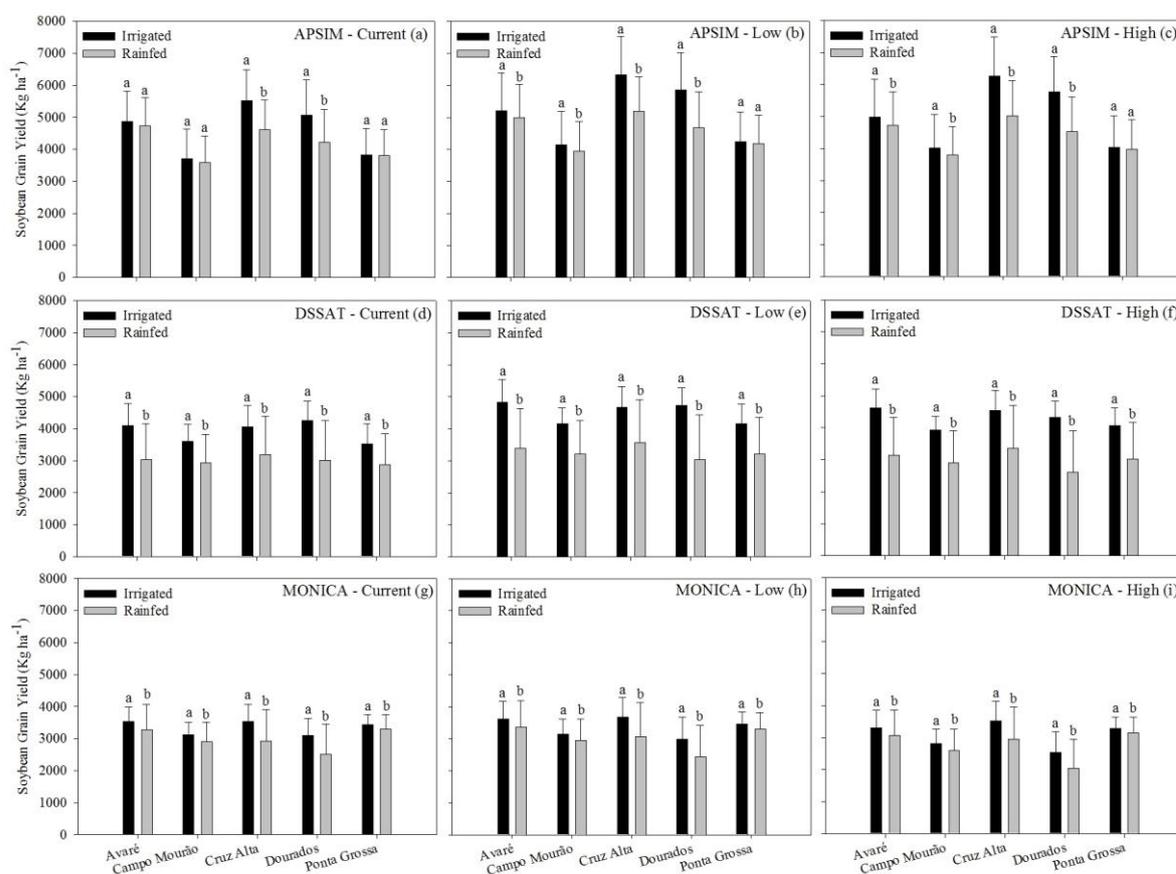


Figure 1 – Soybean grain yield under supplementary irrigation and rainfed conditions for current (a, d and g), low (b, e and f) and high sensitivity (c, f and i) in future climate scenarios simulated by APSIM (a, b and c), DSSAT (d, e and f) and MONICA (g, h and i) crop models for five sites in Southern Brazil. Bars with same letter for each site and climate are not significantly different as determined by Tukey test at the 5% level. The range showed in the bars is the standard deviation. Values are means of 53 crop seasons for the maturity group 6.8 and plant density of 30 plants m⁻²

5.3.2.2 Sowing Dates

Relative to sowing date, the main tendency obtained by the APSIM model was a reduction of yield corresponding to a delay of sowing from 15 Sep to 15 Jan, under conditions

observed in the baseline and the two future scenarios (see the results for Cruz Alta, Figure 2), following a very similar tendency as crop cycle duration as a function of sowing date (Figure 2g and 2h). For DSSAT, the model simulated an increase in yield from 15 Sep to 15 Nov, when yield peaked, and after declined with sowing date until 15 Jan (Figure 2). The delay from the date of 15 Nov to 15 Jan causes greater yield reduction than sowing earlier than 15 Nov for all scenarios, while under rainfed conditions, the yield differences between sowing dates were smaller, when compared to irrigated conditions (Figure 2). For the MONICA model, under current climate and irrigated conditions, all sites showed a slight reduction from 15 Sep until 15 Dec, and an even slighter increase from 15 Dec to 15 Jan. Under rainfed conditions, this tendency was observed only for Cruz Alta, Ponta Grossa and Campo Mourão, while Avaré and Dourados experience a reduction in simulated yields from 15 Sep to 15 Jan, the same tendency observed under future climate scenarios in most cases.

The yield response simulated by each crop model differs along sites and is a function of model characteristics, parametrization and calibration (ASSENG et al., 2013; MARTRE et al., 2015; VAN BUSSEL et al., 2016) and also the yield variability attributed to the rainfall distribution and soil water availability in Southern Brazil (FARIAS et al., 2001; BERGAMASCHI et al., 2007). Based on the results from the ensemble of models, the tendency was similar between climate scenarios, as demonstrated through relative soybean yields (Figure 3). It is possible to verify that the use of supplementary irrigation stabilizes yields across sowing dates. Under rainfed conditions, the variability in yield is a function of rainfall amount (BANNAYAN et al., 2013), a climate variable that was not changed within scenarios, which results in this tendency being similar between the current and future climate scenarios.

According to the ensemble of models, yields tend to reduce from 15 Sep to 15 Jan (Figure 3). The sowing dates from 15 Sep to 15 Nov resulted in most years showing yields above average for all climatic conditions, but although sowing 15 Sep had a similar median yield as 15 Oct, the latter produced more stable yields, especially under climate change under both water management options. Do Rio et al. (2015) simulated soybean yields for South Brazil under different periods and future climate, also concluding that a delay in sowing from the period between 21 Oct and 10 Nov to between 11 Nov and 30 Nov can improve yields. These results are different from the ensemble observed in our study, but Do Rio et al. (2015) used only one crop model (DSSAT), considering also changes in rainfall, but not for [CO₂] on the soybean crop under future scenarios.

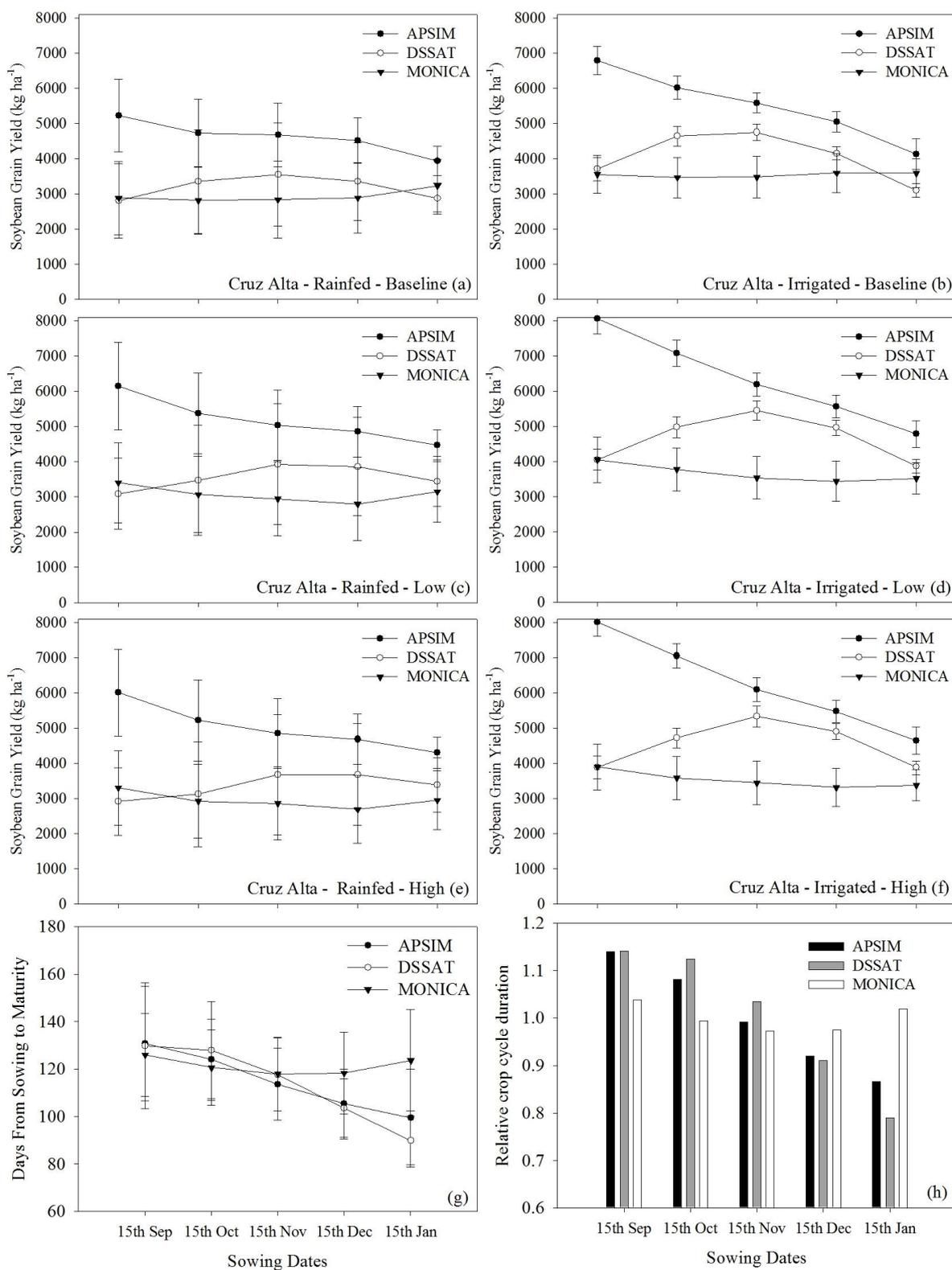


Figure 2 – Soybean grain yield under rainfed (a, c and e) and irrigated (b, d and f) conditions for the baseline (a and b), low (c and d) and high (e and f) future climate scenarios for Cruz Alta, RS, and crop cycle in function of sowing date (g and h) for five sites in Southern Brazil simulated by APSIM, DSSAT and MONICA

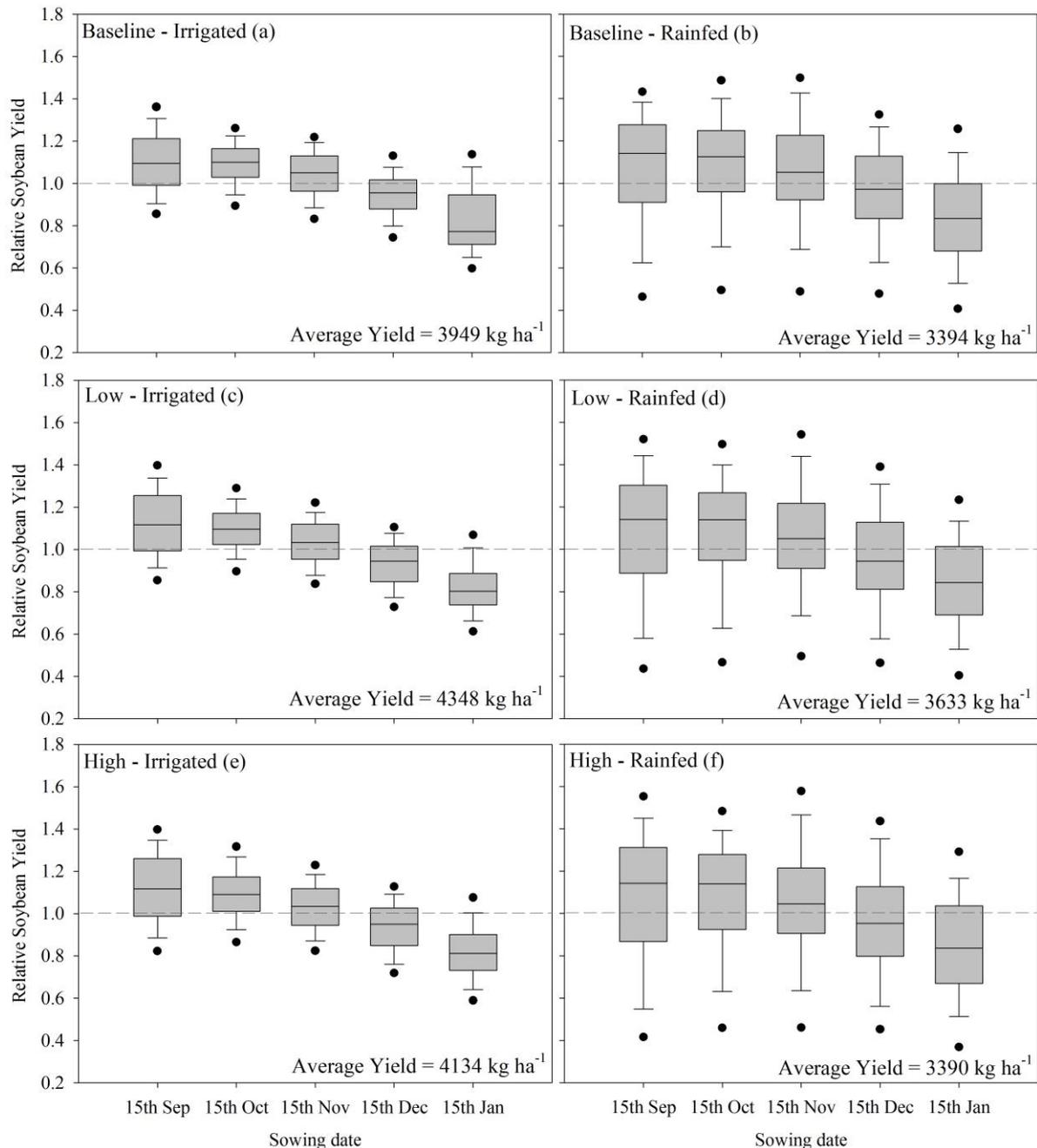


Figure 3 – Relative soybean yield simulated under irrigated (a, c and e) and rainfed (b, d and e) conditions for the baseline (a and b), low (c and d) and high (e and f) future climate scenario. The values were obtained from the ensemble of three crop models and five sites, where the relative soybean yield was obtained dividing the result from each crop season by the mean of whole series for each set of crop model, climate scenario and site results

5.3.2.3 Maturity Group

The simulations showed interactions between water management and maturity group, with difference responses among the crops models (Figure 4). The APSIM model produced

similar responses of maturity group, water management (irrigated and rainfed) and climate scenarios (Figure 4a and 4b), with an increase of yield from maturity group 5.8 to 7.8. Rurinda et al. (2015) found that cultivar cycles (short, medium and long) did not generate different yield results for maize simulated in climate change scenarios in Southern Africa. This was attributed to the difference between short and long cultivars only being 11 days to the time of maturity. In the simulations performed by APSIM, the differences in time of maturity were around 15 and 35 days, respectively, between maturity groups 7.8 and 6.8, and 7.8 and 5.8, and the model simulated lower water deficit than the other models due to greater root density.

In the DSSAT model, the simulations indicated a superior yield for maturity group 7.8 under the baseline climate with irrigation, while 7.8 was similar to 6.8 under rainfed conditions (Figure 4). Under the future scenarios, maturity group 6.8 was better than 7.8 in all climates and water managements, while maturity group 5.8 had the lowest yields. Maturity group 6.8 was more productive under climate change because of the longer cycle than maturity group 5.8, due to conditions that improve yield (KUMAGAI; SAMESHIMA, 2014), but required less total water over its cycle than maturity group 7.8 (SPEHAR et al., 2015). In this context, Rurinda et al. (2015) reached a similar conclusion, in that a short-cycle cultivar with greater drought tolerance can help to stabilize yields in the future, while Bao et al. (2015) observed that some soybean cultivars were more appealing than others under rainfed conditions and future climate.

In comparison to the other models, MONICA results had maturity group 5.8 producing the highest yields for all climate scenarios under irrigated and rainfed conditions (Figure 4). Contrasting with the MONICA results, Kumagai and Sameshima (2014) observed that a cultivar with a longer flowering period and, consequently, longer complete cycle, had higher yield, due to increased leaf area, photosynthesis and number of flowers, pods and seeds. This was not observed when using MONICA model because the maximum effective root depth was limited to 0.75 m during the calibration, a condition that led to increased yield penalization by water deficit in the longer cycles of maturity groups 6.8 and 7.8 (SPEHAR et al., 2015).

The interaction between maturity group and sowing date is a function of environmental and crop cycle characteristics (BASTIDAS et al., 2008; SPEHAR et al., 2015; BAO et al., 2015), as showed in Table 3, 4 and 5. Using the APSIM model, the highest yield was obtained for maturity group 7.8, followed by 6.8 and then 5.8, for all sowing dates and climate scenarios. The interaction only occurred for Cruz Alta, where maturity groups 6.8 and

7.8 had similar yields and were superior to maturity group 5.8 for most sowing dates and climatic conditions (Table 3), except for the sowing dates of 15 Dec and 15 Jan for the future climate, for which 7.8 was superior to 6.8, as was 6.8 to 5.8.

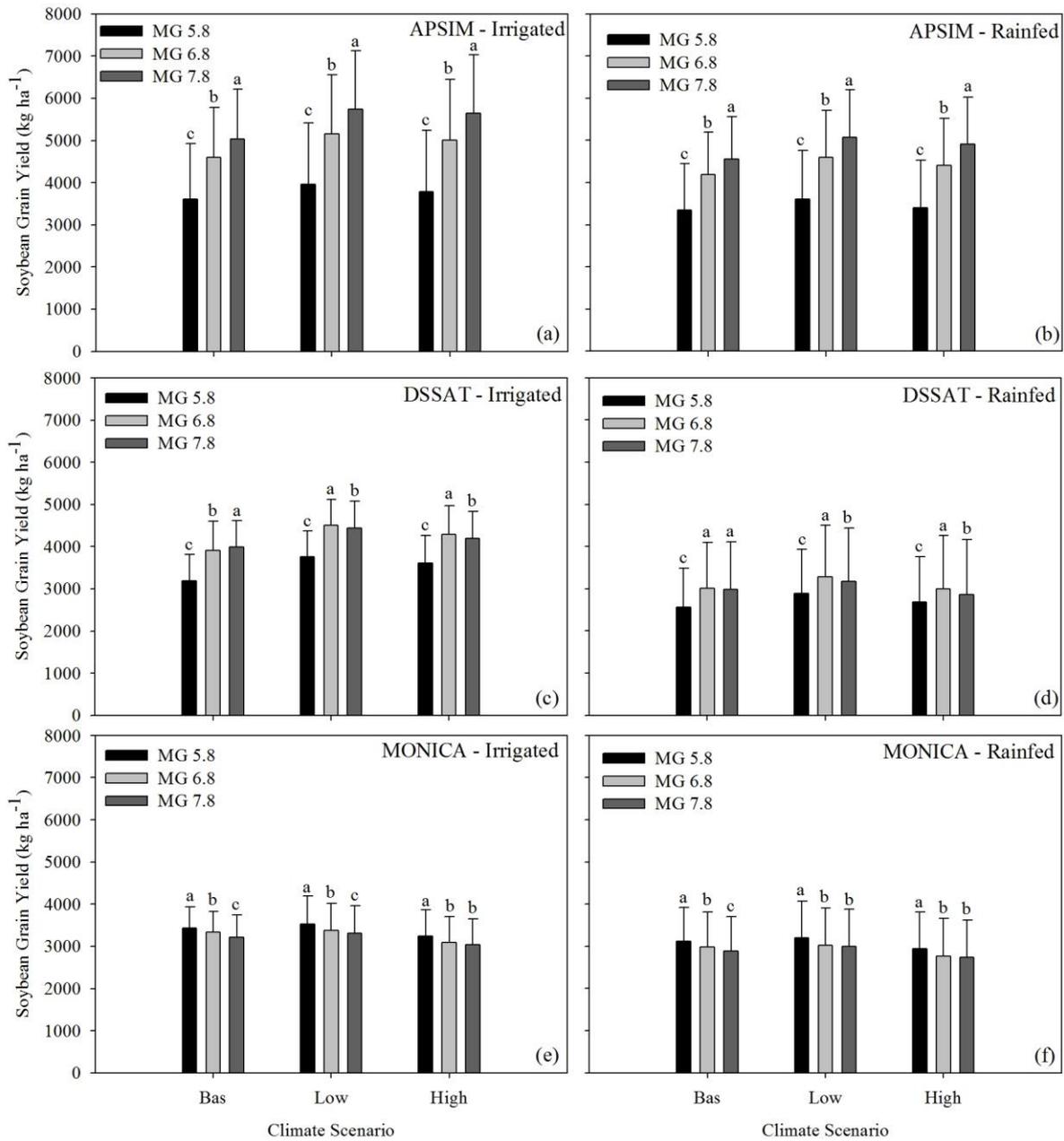


Figure 4 – Soybean grain yield simulated for the maturity groups (MG) 5.8, 6.8 and 7.8 under irrigated (a, c and e) and rainfed (b, d and f) conditions by the crop models APSIM (a and b), DSSAT (c and d) and MONICA (e and f). The values are from the mean of five sites

Table 3 – Soybean grain yield for different maturity groups (MG), climate scenarios and sowing dates simulated by APSIM crop model for five sites in Southern Brazil

MG	Bas					Low					High				
	Sowing date					Sowing date					Sowing date				
	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th
Cruz Alta															
5.8	5780 b	5291 b	4625 b	4152 b	3233 b	6579 b	6085 a	5035 b	4349 c	3447 c	6362 b	5953 b	4884 b	4132 c	3235 c
6.8	6007 ab	5373 ab	5127 a	4783 a	4031 a	7108 a	6231 a	5617 a	5214 b	4634 b	7009 a	6136 ab	5471 a	5079 b	4474 b
7.8	6186 a	5636 a	5341 a	4911 a	3968 a	7292 a	6441 a	5872 a	5449 a	4803 a	7171 a	6354 a	5726 a	5328 a	4742 a
Ponta Grossa															
5.8	3756 c	3755 c	3172 c	2515 c	1743 c	3899 c	4084 c	3154 c	2502 c	1818 c	3477 c	3816 c	2965 c	2269 c	1602 c
6.8	4681 b	4322 b	4036 b	3494 b	2548 b	5298 b	4849 b	4240 b	3665 b	2991 b	5089 b	4771 b	4035 b	3399 b	2732 b
7.8	5012 a	4627 a	4336 a	3838 a	2726 a	5805 a	5203 a	4631 a	4238 a	3563 a	5691 a	5180 a	4508 a	4068 a	3407 a
Campo Mourão															
5.8	3083 c	3433 c	2675 c	2088 c	1472 c	3189 c	3800 c	3094 c	2380 c	1701 c	2915 c	3629 c	3015 c	2280 c	1619 c
6.8	4559 b	4334 b	3721 b	3135 b	2508 b	4978 b	4953 b	4065 b	3450 b	2807 b	4737 b	4853 b	3952 b	3334 b	2651 b
7.8	5224 a	4695 a	4169 a	3817 a	3076 a	5887 a	5442 a	4655 a	4198 a	3545 a	5730 a	5379 a	4593 a	4078 a	3355 a
Avaré															
5.8	4673 c	4765 c	3795 c	3068 c	2326 c	4497 c	4948 c	3997 c	3204 c	2392 c	4066 c	4607 c	3831 c	3004 c	2213 c
6.8	5971 b	5348 b	4760 b	4232 b	3659 b	6353 b	6031 b	5052 b	4398 b	3686 b	6009 b	5880 b	4817 b	4154 b	3395 b
7.8	6490 a	5695 a	5102 a	4680 a	4140 a	7186 a	6574 a	5561 a	5046 a	4429 a	6924 a	6484 a	5484 a	4910 a	4161 a
Dourados															
5.8	4348 c	4421 c	3577 c	2997 c	2326 c	4638 c	5041 c	4215 c	3603 c	2823 c	4464 c	4947 c	4139 c	3564 c	2793 c
6.8	5803 b	5305 b	4515 b	4054 b	3566 b	6410 b	6077 b	5172 b	4646 b	4023 b	6208 b	5910 b	5099 b	4581 b	3922 b
7.8	6405 a	5814 a	5032 a	4625 a	4187 a	7280 a	6650 a	5696 a	5189 a	4622 a	7067 a	6436 a	5524 a	5046 a	4488 a

¹Bas= Baseline for the current conditions (1961-2014); and the future projections for low and high sensitivity in the climate model; ²The means followed by the same letters in the column for each site and sowing date were not significantly different as determined by Tukey test at the 5% level. Values are means of 53 crop seasons for the maturity group 6.8 and plant density of 30 plants m⁻²

Table 4 – Soybean grain yield using different maturity groups (MG), climate scenarios and sowing dates simulated by DSSAT crop model for five sites in Southern Brazil

MG	Bas					Low					High				
	Sowing date					Sowing date					Sowing date				
	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th
Cruz Alta															
5.8	3048 a	3508 b	3862 a	3427 b	2534 b	3662 a	3898 a	4458 a	4058 b	3183 b	3562 a	3670 a	4240 a	3963 a	3167 b
6.8	3249 a	3991 a	4146 a	3747 a	2980 a	3576 a	4227 a	4695 a	4413 a	3655 a	3400 a	3924 a	4503 a	4292 a	3632 a
7.8	3081 a	3773 ab	4027 a	3805 a	3079 a	2952 b	3889 a	4396 a	4411 ab	3811 a	2693 b	3634 a	4218 a	4287 a	3785 a
Ponta Grossa															
5.8	2413 b	2945 b	3214 b	2759 b	1855 c	2826 b	3243 b	3649 b	3284 b	2330 c	2681 b	3064 b	3490 b	3201 b	2312 c
6.8	3003 a	3697 a	3778 a	3223 a	2319 b	3444 a	3980 a	4309 a	3811 a	2885 b	3320 a	3726 a	4128 a	3707 a	2834 b
7.8	2927 a	3687 a	3772 a	3382 a	2511 a	3021 b	3840 a	4174 a	3973 a	3140 a	2843 b	3548 a	4006 a	3838 a	3103 a
Campo Mourão															
5.8	2549 c	2978 b	3157 b	2743 b	1961 c	2778 c	3291 b	3564 b	3248 b	2471 c	2571 b	3008 b	3288 b	3117 b	2425 b
6.8	3296 a	3611 a	3742 a	3240 a	2473 b	3599 a	3857 a	4192 a	3762 a	3009 b	3262 a	3477 a	3863 a	3557 a	2908 a
7.8	2932 b	3574 a	3823 a	3430 a	2722 a	3111 b	3593 a	4128 a	3918 a	3239 a	2781 b	3158 b	3784 a	3664 a	3093 a
Avaré															
5.8	2562 b	3190 b	3432 b	2816 b	1858 c	2773 b	3570 b	3977 b	3407 b	2404 c	2568 b	3316 b	3759 b	3286 b	2399 c
6.8	3578 a	4185 a	4161 a	3467 a	2437 b	3972 a	4627 a	4795 a	4094 a	3056 b	3651 a	4254 a	4523 a	3938 a	3007 b
7.8	3553 a	4418 a	4416 a	3707 a	2763 a	3894 a	4628 a	4967 a	4368 a	3376 a	3557 a	4166 a	4662 a	4188 a	3290 a
Dourados															
5.8	2919 c	3266 b	3484 b	3099 b	2354 c	3171 b	3480 b	3800 a	3600 b	2919 b	2911 b	3077 ab	3358 a	3322 a	2834 b
6.8	3816 a	3955 a	3953 a	3550 a	2881 b	3936 a	3922 a	4216 a	3921 ab	3420 a	3483 a	3347 a	3674 a	3603 a	3255 a
7.8	3474 b	3649 a	3867 ab	3710 a	3136 a	3382 b	3364 b	3871 a	4038 a	3593 a	2852 b	2762 b	3354 a	3645 a	3382 a

¹Bas= Baseline for the current conditions (1961-2014); and the future projections for low and high sensitivity in the climate model; ²The means followed by the same letters in the column for each site and sowing date were not significantly different as determined by Tukey test at the 5% level. Values are means of 53 crop seasons for the maturity group 6.8 and plant density of 30 plants m⁻²

Table 5 – Soybean grain yield using different maturity groups (MG), climate scenarios and sowing dates simulated by MONICA crop model for five sites in Southern Brazil

MG	Bas					Low					High				
	Sowing date					Sowing date					Sowing date				
	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th	Sep 15th	Oct 15th	Nov 15th	Dec 15th	Jan 15th
Cruz Alta															
5.8	3447 a	3366 a	3365 a	3346 a	3533 a	4024 a	3704 a	3528 a	3401 a	3366 a	3871 a	3520 a	3357 a	3267 a	3220 a
6.8	3215 ab	3137 a	3155 ab	3239 a	3408 a	3730 ab	3424 ab	3247 ab	3123 b	3335 a	3599 ab	3254 ab	3151 ab	3000 ab	3160 a
7.8	3160 b	3092 a	3051 b	3334 a	2630 b	3607 b	3279 b	3030 b	3094 b	3313 a	3453 b	3118 b	2904 b	2963 b	3174 a
Ponta Grossa															
5.8	3502 a	3415 a	3385 a	3332 b	3410 a	3715 a	3580 a	3451 a	3298 a	3275 a	3588 a	3437 a	3267 a	3170 a	3109 a
6.8	3360 ab	3311 a	3303 a	3365 ab	3463 a	3604 a	3417 b	3360 ab	3215 a	3305 a	3422 a	3293 b	3171 ab	3082 a	3101 a
7.8	3340 b	3322 a	3319 a	3456 a	2641 b	3571 a	3397 b	3287 b	3262 a	3319 a	3434 a	3280 b	3139 b	3063 a	3155 a
Campo Mourão															
5.8	3299 a	3190 a	3007 a	2864 a	2934 a	3473 a	3349 a	3160 a	2905 a	2866 a	3154 a	3014 a	2841 a	2654 a	2555 a
6.8	3213 a	3049 b	2892 ab	2861 a	3025 a	3393 a	3201 ab	2973 b	2819 a	2814 a	3020 a	2835 b	2647 b	2535 a	2506 a
7.8	3127 a	2931 b	2833 b	2912 a	3040 a	3458 a	3133 b	2897 b	2806 a	2871 a	3113 a	2773 b	2597 b	2504 a	2521 a
Avaré															
5.8	3888 a	3739 a	3511 a	3331 a	3250 a	4039 a	3942 a	3712 a	3424 a	3206 a	3723 a	3623 a	3375 a	3172 a	2882 a
6.8	3732 a	3555 b	3363 b	3203 a	3166 ab	3913 a	3783 ab	3539 b	3241 b	2974 b	3604 a	3454 ab	3210 b	2975 b	2714 a
7.8	3677 a	3451 b	3295 b	3170 a	2941 b	3954 a	3747 b	3453 b	3124 b	2961 b	3640 a	3403 b	3218 b	2869 b	2700 a
Dourados															
5.8	3337 a	3122 a	2969 a	2764 a	2616 a	3399 a	3250 a	2963 a	2668 a	2431 a	2928 a	2796 a	2450 a	2249 a	2041 a
6.8	3148 ab	2919 ab	2792 ab	2609 a	2541 a	3290 a	2943 b	2701 b	2385 b	2239 a	2798 a	2494 b	2245 b	2008 b	1911 a
7.8	3002 b	2873 b	2627 b	2525 a	2601 a	3227 a	2864 b	2586 b	2290 b	2247 a	2788 a	2440 b	2154 b	1942 b	1898 a

¹Bas= Baseline for the current conditions (1961-2014); and the future projections for low and high sensitivity in the climate model; ²The means followed by the same letters in the column for each site and sowing date were not significantly different as determined by Tukey test at the 5% level. Values are means of 53 crop seasons for the maturity group 6.8 and plant density of 30 plants m⁻²

Using the DSSAT model, the most uncertainty about the best maturity group occurred in early, 15 Sep and 15 Oct, and later, 15 Jan, sowings (Table 4), when the differences in cycle duration between maturity groups increased due to photoperiod sensitivity (SPEHAR et al., 2015). With intermediate sowing dates, in most cases, the maturity groups 6.8 and 7.8 had higher yields than 5.8. This interaction between maturity group and sowing date also was observed by Bao et al. (2015), where later-sowed soybeans showed a larger increase in yield than those sowed earlier; however for a cultivar with a longer growing season, earlier sowing was better because longer cycle increased risk of frost damage in Southeastern USA.

The maturity groups 5.8 and 6.8 were similar ($p < 0,05$) when using the MONICA crop model, for all sowing dates in Cruz Alta, Ponta Grossa and Dourados, and most sowing dates for Campo Mourão and Avaré, under current climatic conditions (Table 5). Under the same climatic conditions, maturity group 7.8 was similar to 5.8 and 6.8 at Ponta Grossa for sowings between 15 Oct and 15 Dec, at Campo Mourão for 15 Sep, 15 Dec and 15 Jan, and in Dourados for 15 Dec and 15 Jan. For the future scenarios, the maturity group 5.8 presented superior yields in all cases when simulated by MONICA model. This probably occurred due to the increase of temperature leading to greater water demand and the early-maturity cultivars suffering less under drought than those of longer cycles (SPEHAR et al., 2015).

5.3.2.4 Plant Density

Plant density management was simulated using the crop models APSIM and DSSAT. The results were similar for both crop models when evaluating the more productive plant population for each site. In Cruz Alta, both models indicated that the plant population of 30 and 50 plants m^{-2} were similar ($p < 0.05$) and superior to 10 plants m^{-2} (Data not shown) for all climate scenarios. In Dourados, the results were similar to Cruz Alta, except for the simulation performed by DSSAT, which indicated that the population of 30 plants m^{-2} was similar to 50 plants m^{-2} only under future climates. For these sites, the results indicated that an increase in sowing density resulted in a higher crop water demand due to greater leaf area (ALLEN et al., 1998), resulting in similar performances of 30 and 50 plants m^{-2} . In the population of 10 plants m^{-2} the lower leaf area does not enable the potential yield of soybean (MAYERS et al., 1991) and it can increase soil evaporation, reducing the water availability to the crop (SAUER et al., 2007). For the other sites, denser population (50 plants m^{-2}) showed better performance than medium (30 plants m^{-2}) and lower (10 plants m^{-2}) densities, with the same tendency across all climate scenarios. The higher sowing density provided a faster leaf

area development and earlier canopy closure, improving the solar radiation interception (BOOTE; PICKERING, 1994), although it can lead to increased risk of lodging (MAYERS et al., 1991).

The models had different yield levels resulting from plant density, with higher yields for 50 plants m^{-2} , with similar values for 30 plants m^{-2} , while 10 plants m^{-2} had lower yield by the greatest difference (Figure 5). This tendency was similar for the climate scenarios, but the difference between plant populations increased at the extremes of the sowing window (15 Sep and 15 Jan), while in the middle, between 15 Oct and 15 Dec, the difference between plant populations was lower. Mayers et al. (1991) observed that adjusting correctly the sowing date can improve the plant growth and the leaf area index for lower plant populations. In present study, better sowing dates for soybean occurred between 15 Oct and 15 Dec, resulting in lower difference of yield between 10, 30 and 50 plants m^{-2} .

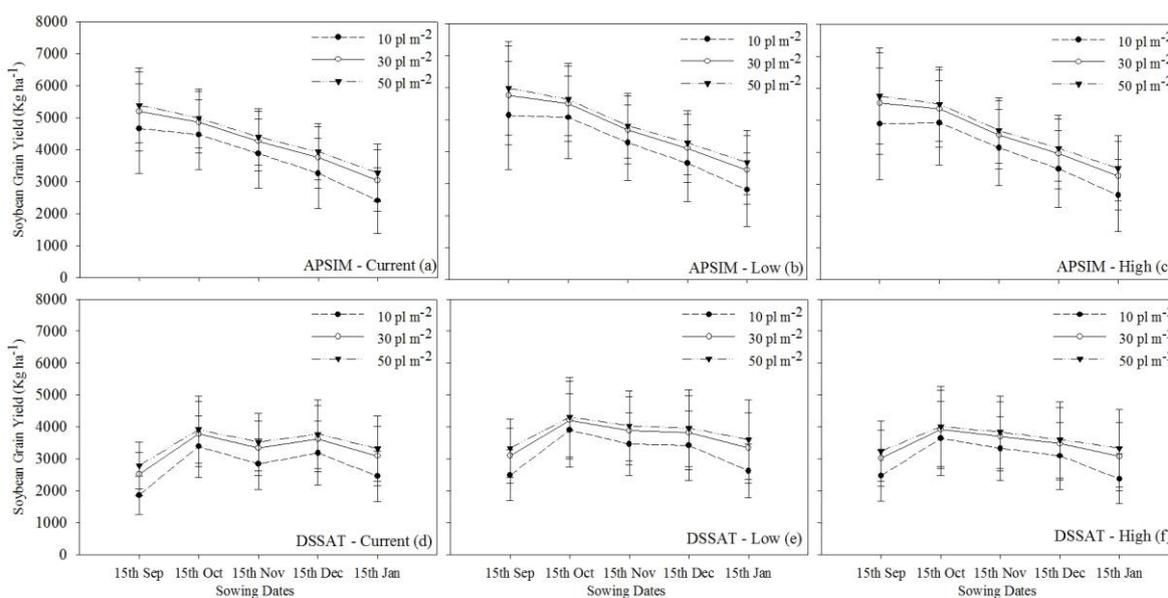


Figure 5 – Soybean grain yield simulated under different plant populations by APSIM (a, b and c) and DSSAT (d, e and f) crop model for three climate scenarios in five sowing dates in Southern Brazil. The values are from the mean of five sites

5.4 Conclusions

The crop models simulated different yield levels for crop management and sites evaluated under different climate conditions in the Southern Brazil. Supplementary irrigation helped to create higher and more stable yields throughout the crop seasons, with greater yield gains under future climate than current, due to CO₂ fertilization and dryer conditions

conducive to irrigation. Sowing dates presented different tendencies by crop models, but within the model ensemble, response to all climate scenarios were similar, with a reduction of yield from 15 Sep to 15 Jan, which was more intense from 15 Nov to 15 Jan. Maturity groups had no clear tendency between the models, but showed that if conditions tend to be dryer, the short maturity group (5.8) is a better option than a late-ripening cultivar (7.8), which is better under conditions with sufficient soil water availability. Denser plant populations always had higher yields for all climate scenarios, but needs to be evaluated carefully due to other factors, such as the increased risk of lodging that can result from plant density and cause yield losses. In this way, crop management does not demonstrate clear potential in the shift from current to future scenarios to increase the crop resilience to climate change. These results must be considered to be associated with rain patterns as a limiting factor of yield, an important variable that was not changed in simulated future climates, while air temperature is not limiting factor for soybean considering the historic weather records and the projections for the future in Southern Brazil.

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6 GENERAL CONCLUSIONS

Based on the results obtained in this study and answering the aims proposed, it is possible to conclude:

- All crop models were able to simulate efficiently yield and crop phases to soybean in the region after calibrated the coefficients related with crop development, growth and related with soil, capturing different levels of yield in the sites of field experiment under rainfed and irrigated conditions. It was observed that for all models was necessary to adjust coefficients related with soil that affect root water uptake, being a limiting point in the calibration that need to be analysis carefully. For the results obtained in the simulation yield, using independent data, it was observed a poor performance, which occurred because of factors not consider by model, as diseases, and limited information about soil and climate specific from the sites of field experiment, committing model performance.

- Based in the models performance, the choice of crop model to use in simulation of soybean growth can be done based on the capacity of model to attend the objective of study and accessible of information and knowledge of user to calibrate and use the model, independently of model complexity. Other point it is very recommended the use of the results from crop models ensemble, which had the best performance than the best single crop model.

- Crop models were sensitivity to changes in air temperature, [CO₂], solar radiation and rainfall. In most cases, crop models simulated a reduction of soybean yield when the air temperature was increased, what was caused by a shorter crop cycle in relation to the baseline data and the crop model approach used to estimate crop development, mainly associated to the cardinal temperatures considered by each of them. When rainfall was changed, the models simulated higher yield reductions due to lower rainfall amount than the yield increase with more rainfall. Solar radiation changes had yield response different by site and crop models, due to interaction between potential yield (positively) and evapotranspiration (negatively). The relative yield gains were higher under lower [CO₂] increase (+100 ppm) than under higher increase (+400 ppm), for all models, which was a consequence of the similar asymptotic response curve that all models use for CO₂ assimilation. Combining all climate changes, the models showed that the benefits of increased [CO₂] for soybean yield can compensate the negative effect of increased air temperature; therefore, the present results show that soybean yield was more affected by associated changes on rainfall and solar radiation.

- In the simulation, it is interesting to analyze the intermediate processes, especially under climate change simulation. For example, when considered increase of rainfall amount that increased runoff and deep drainage, or the secondary effect of [CO₂] on stomatal conductance and consequently on transpiration. So, it requires more attention from modelers in order to improve models for simulating more accurately the future scenarios

- Different traits evaluated can help to improve soybean yield under current and future climates in order to develop cultivars with adaptation to drought for Southern Brazil. All traits showed a greater yield gain in the future climate than current climate. Deeper root depth was the most promising among all traits. Traits that create a better root distribution in the soil, greater root mass allocation under water deficit, reduce transpiration with lower penalization in photosynthesis, promote nitrogen fixation drought tolerance, and reduced acceleration of grain filling period in response to water deficit have potential to be included alone or together (potentiated effect) in new cultivars for the Southern Brazil.

- The crop models simulated different yield levels for crop management and sites evaluated under different climate conditions in the Southern Brazil. Crop management does not demonstrate clear potential in the shift the best option from current to future scenarios to increase the crop resilience to climate change. These results must be considered to be associated with rain patterns as a limiting factor of yield, variable that was not changed in simulated future climates.

- The simulation of future climate conditions need to be analyze based on current climate and the limiting yield aspects. In the Southern Brazil, the air temperature was not a limiting factor for soybean considering the historic weather records and the projections for the future, but is necessary to consider that cardinal temperature and approach used in crop development cannot be correct, especially the maximum values that are the mainly difference between the models, requiring experiment results considering high values of air temperature and the effect on crop cycle.

- Crop models showed to be an interesting tool to be used, if associated with field experiment, to evaluate crop management, as such irrigation, sowing date, cultivar and plant density, as well as, to create virtual cultivars with adaptation to drought and other traits for different environmental conditions, considering that the crop model are able to simulate the processes require to represent correctly the crop management or the trait of interest.

APPENDIX

Appendix A – Experimental Details

The size of plots and number of replications and subsamples were based on information compiled from the following studies: Estefanel et al. (1984); Martin et al. (2005); Martin et al. (2007); Cargnelutti Filho et al. (2009); Cargnelutti Filho and Gonçalves (2011). Three replicates were used for sowing date, in which plots 1 and 2 had seven planting rows and the third, eight planting rows. The three replicates were sown in sequence one beside the other, totaling 22 planting rows, as presented in Figure 1, with sowing lines used as boundary, which were used for growth analysis during crop development and for yield analysis in the end of cycle. In the sowing row used to growth analysis, a boundary of 0.5 m from the beginning of the row to the point where the sample was collected was left, keeping the same boundary for the next sample made in the row. This experimental design was adopted assuming that soil characteristics of the field are homogeneous. Furthermore, the adoption of any other type of design would influence the results of the next sowing dates associated with the plant height from first sowing. Sowing was made in the north-south orientation, in order the highest plants from the first sowing date did not project shadow to the other plants, from subsequent sowings.

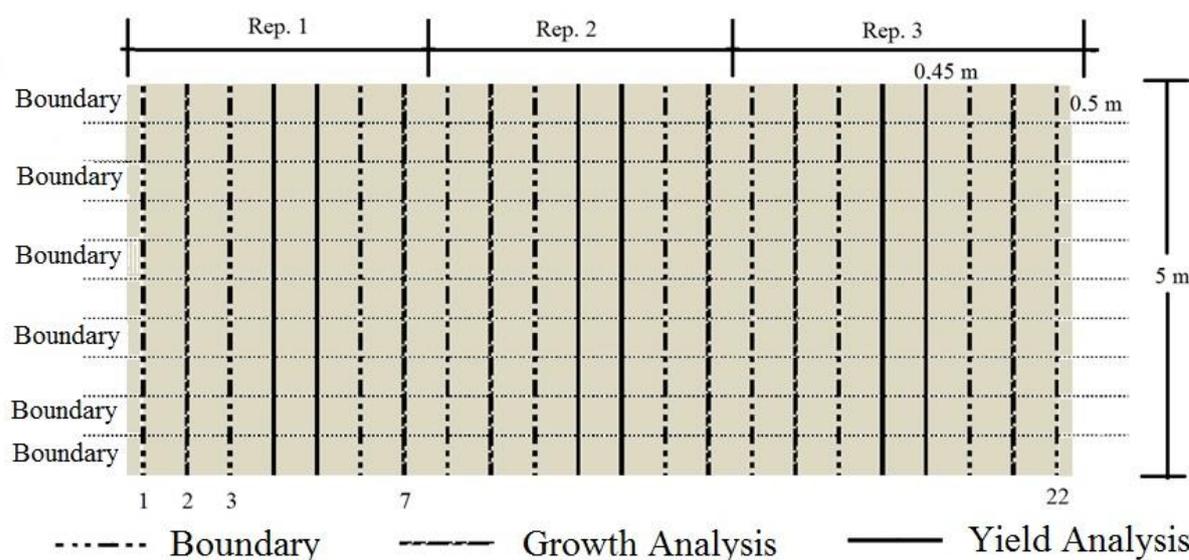


Figure 1 – Schematic of the field experiment design with sowing lines used as boundary and for growth and yield analysis

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Appendix B – Soil details in experiments

Soil physical and chemical conditions were measured using 10 subsamples collected in each experimental area to create a mean sample. Soils were sampled at 0-0.15, 0.15-0.30 and 0.30-0.50 m depth in Piracicaba and Frederico Westphalen, and at 0-0.20 and 0.20-0.40 and 0-0.10, 0.10-0.20 and 0.20-0.30 m depth in Londrina, respectively for chemical and physical analysis (Tables 1, 2 and 3). Chemical samples were collected using a shovel, while for the physical analysis a cylinder with $\pm 100 \text{ cm}^3$ was used. Data measured were macronutrients and micronutrients, organic matter, pH, sand, clay and silt. Soil cylinder were used to determine the saturation, field capacity (-10 kPa) and wilting point (-1500 kPa), bulk density and saturated conductivity.

Table 1 – Chemical and physical soil (Nitossolo Vermelho) conditions in Piracicaba, SP

Layer (m)	pH	P	K	MO	Al	Ca	Mg	CEC
		mg L ⁻¹		%	cmol L ⁻¹			
0.0-0.15	5.60	8.50	183.50	1.70	0.00	3.20	1.10	7.80
0.15-0.30	5.50	8.30	181.00	1.70	0.00	3.30	1.30	7.80
0.30-0.50	5.50	5.80	77.50	1.40	0.00	3.20	1.30	7.40
Layer (cm)	H+Al	% Sat. of CTC		S	Zn	Cu	B	Mn
	cmol L ⁻¹	Bases	Al	mg L ⁻¹				
0.0-0.15	3.00	61.40	0.00	20.00	7.10	7.10	0.50	14.00
0.15-0.30	2.70	65.20	0.00	23.90	6.90	7.60	0.50	11.00
0.30-0.50	2.70	63.50	0.00	29.50	3.30	7.30	0.30	8.00
Layer (m)	Clay	Silt	Sand	BD	Sat	DUL	LL	Ksat
	%			Mg m ⁻³	cm cm ⁻³		mm min ⁻¹	
0.0-0.15	55.80	14.30	29.90	1.36	0.63	0.43	0.25	1.81
0.15-0.30	57.80	13.30	29.00	1.41	0.60	0.43	0.26	0.73
0.30-0.50	63.80	10.80	25.40	1.52	0.57	0.47	0.26	0.86

BD= bulk density; Sat= soil saturation; DUL= drainage upper limited; LL= lower limited; Ksat= conductivity saturation

Table 2 – Chemical and physical soil conditions for a Ferralsol (Latosolo Vermelho) in Frederico Westphalen, RS, Brazil

Layer (m)	pH	P	K	MO	Al	Ca	Mg	CEC
		mg L ⁻¹		%	cmol L ⁻¹			
0.0-0.15	5.30	30.50	231.00	2.70	0.20	4.30	2.10	11.30
0.15-0.30	5.80	3.40	139.50	2.00	0.00	4.00	1.50	12.00
0.30-0.50	4.90	3.50	89.00	1.60	0.90	2.90	1.80	8.80
Layer (m)	H+Al	%Sat. da CTC		S	Zn	Cu	B	Mn
	cmol L ⁻¹	Bases	Al	mg L ⁻¹				
0.0-0.15	4.30	61.90	2.80	11.90	5.20	7.60	0.30	51.00
0.15-0.30	3.60	70.00	0.00	23.00	1.40	8.20	0.20	34.00
0.30-0.50	3.90	55.80	15.40	25.90	2.50	8.90	0.20	35.00
Layer (m)	Clay	Silt	Sand	BD	Sat	DUL	LL	Ksat
	%			Mg m ⁻³	cm cm ⁻³		mm min ⁻¹	
0.0-0.15	75.40	16.20	8.40	1.21	0.58	0.47	0.30	0.09
0.15-0.30	77.40	15.30	7.20	1.22	0.58	0.48	0.28	0.03
0.30-0.50	81.40	11.60	7.00	1.19	0.62	0.51	0.29	0.15

BD= bulk density; Sat= soil saturation; DUL= drainage upper limited; LL= lower limited; Ksat= conductivity saturation

Table 3 – Chemical and physical soil conditions for a Ferralsol (Latosolo Vermelho) in Londrina, PR, Brazil

Layer (m)	pH	P	K	MO ¹	Al	Ca	Mg	CEC
		mg L ⁻¹		%	cmol L ⁻¹			
0.0-0.20	4.97	12.90	277.00	2.72	0.00	4.32	1.67	10.80
0.20-0.40	5.15	3.38	160.26	0.90	0.00	4.39	1.68	10.01
Layer (m)	H+Al	%Sat. da CTC		S	Zn	Cu	B	Mn
	cmol L ⁻¹	Bases	Al	mg L ⁻¹				
0.0-0.10	4.10	62.04	0.00	-	-	-	-	-
0.20-0.40	3.53	64.74	0.00	-	-	-	-	-
Layer (m)	Clay ¹	Silt ¹	Sand ¹	BD	Sat	DUL	LL	Ksat
	%			Mg m ⁻³	cm cm ⁻³		mm min ⁻¹	
0.0-0.10	65.00	13.00	22.00	1.28	0.44	0.42	0.30	0.33
0.10-0.20	65.00	13.00	22.00	1.39	0.46	0.45	0.32	0.33
0.20-0.30	65.00	13.00	22.00	1.37	0.48	0.47	0.32	0.33

¹Mean value from Radam Project (1974). BD= bulk density; Sat= soil saturation; DUL= drainage upper limited; LL= lower limited; Ksat= conductivity saturation

Appendix C – Crop growth and development assessment

The methodology used for the assessment of crop phases, in-season (total above dry matter and leaf area index) and end-of-season (yield and harvest index) measurements for soybean are next:

- Development phases: the scale proposed by Fehr and Caviness (1977) was employed, once it is currently used around the world to identify the soybean crop development phases. In the evaluation was determined the date of occurrence of sowing, emergence (VE), beginning of flowering (R1), beginning of pod formation (R3), beginning of grain filling (R5), full grain (R6), beginning of maturity (R7), full maturity (R8) and harvest. The determination of crop phases occurred through periodic visits to the field and the given phase was recorded when at least more than 50% of the portion of useful plants exhibit the characteristics described in Table 1.

Table 1 – Soybean crop stages as defined by Fehr and Caviness (1977)

Periods	Phase	Description
Vegetative	VE	Cotyledons above the soil surface;
	VC	Cotyledons completely open;
	V1	Unifoliate leaf full developed;
	V2	First trifoliate leaf fully open;
	V3	Second trifoliate leaf fully open;
	Vn	Ante-nth trifoliate leaf fully open.
Reproductive	R1	Beginning of bloom – one open flower at any node on the main stem;
	R2	Full bloom – An open flower at one of the two uppermost nodes on the main stem with a fully developed leaf;
	R3	Beginning of pod – Pods are 5 mm at one of the four uppermost nodes on the main stem with a fully developed leaf;
	R4	Full pod – Pods are 2 cm at one of the four uppermost nodes on the main stem with a fully developed leaf;
	R5	Beginning of seed – Pod at one of the four uppermost nodes on the main stem contains seed that are 3 mm long;
	R6	Full seed – pod at one of the four uppermost nodes on the main stem contains green seeds that fill the pod cavity;
	R7	Beginning of maturity – one normal pod on the main stem has reached its mature pod color;
	R8	Full maturity – 95 percent of the pods have reached their full mature color;

Source: Farias et al. (2009)

- Total above dry matter: five plants per replication were sampled at the intervals at 20 day after emergence, beginning of flowering, beginning of pod formation, beginning seed

formation, full seed and after full maturity. The plants were divided in three parts for the analysis of growth: leaf lamina, stem/petiole, and reproductive organs (flowers and pods). After separation of the plant parts, they were placed in paper bags, properly identified, indicating the number of replication, sowing date and plant part, and then dried at ± 60 °C, where they were kept until reached constant weight. After complete drying, the samples were weighed and the results converted to one hectare.

- Leaf area index: it was selected 15 leaf blades per replication, which were placed on a white background to be photographed. Then the “cut-outs” of the photo and the other leaf blades were placed separately in paper bags to dry and then being weighed. Using the relationship between the leaf area and weights of the respective sampled and the total leaf weight, the total leaf area was determined. The leaf area from leaf blade samples was determined using the software QUANT 2002 (VALE et al., 2003). After completing the leaf area determination of, the leaf area index was obtained by dividing total leaf area by the number of plants collected and then by the area occupied by each plant.
- Grain yield: the total grain weight and their residual moisture were determined using plants collected from 3.5 linear meters of the two central rows in each plot, as pre-determined in the scheme of Figure 1 (pg. 157). The yield obtained in the plot area was extrapolated to one hectare based on dry matter of seed. A temperature of 105 °C for a period of 24 h was used to extract the water present in the seed and determine the residual moisture in the sample.
- Harvest Index: this index was determined from the relationship between seed dry weight and total plant dry weight measured immediately after harvest maturity (R8). This harvest index does not consider the leaves lost by natural senescence along the crop cycle.

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Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA

(continued)

Crop Model	Description
Phenology progress rate	
FAO	The model do not simulated crop development, and in the simulation is used the number of days after sowing to define crop development of five stages.
AQUACROP	Uses the thermal time calculated with basal (10°C) and superior (35°C) temperatures for the five stages of development.
DSSAT	It computes phenology based on the photothermal time (temperature x photoperiod). The thermal time is computed based on a curve with the basal, optimum 1 and optimum 2 and maximum temperatures, which is different for each crop phase. For photoperiod is define a value where below it (13 hours), the development rate is maximum (short-day plant), while above this limit the rate is lower than one until reach zero. The rate of progress along the nine stages is also penalization by water deficit and nitrogen limitation in different levels for each crop phase.
APSIM	The model uses the thermal and day length effects based on a curve with four values of day length (x-axis) against four values of thermal time required (y-axis) for the crop to complete each of the nine stages. The thermal time is computed based on a curve with basal, optimum and maximum cardinal temperature. There is also penalization by water deficit and nitrogen limitation with a delay if this occurs between emergence and flowering.
MONICA	The thermal time is computed using one basal temperature that is different for each crop phase, which is penalized by day length factor (0-1). The day length factor is estimated using similar approach to DSSAT. The model has seven stages with their respective thermal time.
Leaf area growth	
FAO	The model use as an input the maximum leaf area index to adjust biomass production from a standard crop.
AQUACROP	Simulates canopy cover, following initial cover, rate of canopy cover growth, maximum cover, beginning and rate of senescence.
DSSAT	Leaf expansion is defined based on the biomass diverged to leaf and specific leaf area. The specific leaf area depends on temperature, light and water deficit. The assimilates sent to leaf is reduced when the crop begins the reproductive growth, and due to nitrogen mobilization photosynthesis declines and leaf abscission starts, which can be accelerated by water deficit. When the crop reaches maturity (R7), all leaves are abscised and seed growth stop.
APSIM	The number of leaves is function of plant node, which is estimate based on thermal time. The potential canopy leaf area is function of potential number of leaf, leaf size per node, plant population and water deficit index to leaf expansion. If there is not enough supply from photosynthesis to leaf growth, the current leaf area will be lower than potential. The supply required is estimated by specific leaf area, which is function of leaf area index and the rate of transformation of dry matter to leaf area. The leaf senescence is the maximum of four values, due to plant age, light competition, water deficit or frost, where the fraction of carbon and nitrogen from senescence part is retranslocated to shoot before the leaf to be lost.

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA

(continuation)

Crop Model	Description
Leaf area growth	
MONICA	The new leaf area index is estimated based on the current leaf area index, the biomass added and lost (senescence) in the current day, specific leaf area at begins and end of current phase, and relative development phase. The senescence is determined by crop phases and begins at first pod.
Photosynthesis and respiration	
FAO	The potential dry biomass is estimated for a pattern crop with leaf area index of 5 based on solar radiation (cloudy and clear sky), air temperature and type of crop (C3 or C4). The temperature also is used to estimate respiration costs, which is a simple approach, 50% of cost if temperature is higher than 20°C, or 40% if is lower than 20°C. The biomass is compute day by day and in end is adjust based on maximum leaf area index coefficient.
AQUACROP	The crop model uses the water use efficiency to estimate total biomass production. The water use efficiency is adjusted as a function of air temperature, through thermal time, and CO ₂ concentration. The total biomass is converted in the final grain yield using carbohydrate conversion efficiency and the composition of grain. Other condition is that if water supply is not enough to supply potential transpiration, photosynthesis is linear penalized by the relationship between actual and potential transpiration. As the model compute final biomass, specific respiration costs is not estimated, once this condition is applied through adjustments in water use efficiency based on air temperature and conversion costs.
DSSAT	The model estimates direct and diffuse (direct converted to diffuse within the canopy, skylight originating from a uniformly-fit sky, and reflected from the soil) solar radiation as function of crop height, leaf area index, leaf angle, sowing direction, latitude, day of year and time of day, defining photosynthetic photon flux to the sunlit and shaded leaves (BOOTE and PICKERING, 1994). The gross photosynthesis follows an asymptotic exponential response to light, based on the quantum efficiency and light-saturated photosynthesis rate in function of CO ₂ , O ₂ and leaves temperature. Light-saturated photosynthesis rate for a single leaf is modelled based on a linear function of specific leaf weight and as a quadratic function of leaf nitrogen, where canopy assimilation is obtained through the sum of all leaves in the plant. The maintenance respiration computed is based on temperature, rate of photosynthesis and current biomass (excepted oil and protein storage in the grains), following McCree (1974). The approach of Penning de Vries and van Laar (1982) is used to compute growth respiration and conversion efficiency for the plant composition defined in the specie coefficients.

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA
(continuation)

Crop Model	Description
Photosynthesis and respiration	
APSIM	The model uses two daily approaches to estimated photosynthesis. First, total dry mass is predicted based on transpiration, using soil water supply multiplied by transpiration efficiency. Transpiration efficiency coefficient is defined by crop phase and vapor pressure deficit. Second, total dry mass is estimated with solar radiation intercepted in function of leaf area index and extinction coefficient (function of row spacing, plant distribution and population), which is convert to dry mass by radiation use efficiency. Total dry mass estimated by radiation use efficiency is also penalized by air temperature, oxygen and nitrogen deficit. The daily biomass will be the smaller value from these two approaches. The model does not consider specific adjustment to crop respiration, once this is included in the coefficients of radiation use efficiency and transpiration efficiency.
MONICA	It uses the model SUCROS (MIRSCHER and WENKEL, 2007) to estimate gross photosynthesis, where the main factors are solar radiation, cloudy and clear sky conditions, air temperature and leaf area index. The respiration cost is computed for the photoperiod (day) and night hours, following AGROSIM (MIRSCHER and WENKEL, 2007). These costs are estimated using the specific maintenance cost from empirical factors, temperature and dry mass of each part of the plant. The maintenance respiration is firstly supplied by current daily photosynthesis assimilates, and secondly is computed cost from growth respiration. This balance is distributed in whole plant.
Biomass partitioning	
FAO	There is no simulation for partitioning to harvest index, being necessary the user to define a value of harvest index as an input.
AQUACROP	The biomass partitioning is only for harvest index, which is estimated based on a potential value and adjusted in function of air temperature and water deficit, condition associated with abortion of flowers. When water deficit occur before of grain filling, there is an increase, and/or if water deficit occur during grain filling period, there is an increase of harvest index if leaf expansion is penalized or a decrease if transpiration is affected.
DSSAT	Assimilates are diverged during vegetative period to leaves, branches and roots in function of each vegetative phase, and water and nitrogen deficit. When crop start reproductive period, the group of pods are added daily based on genetics, temperature, day length, carbon and nitrogen supply. The daily assimilates are distributed, respectively, for seed, podwalls, new pods (daily addition) and vegetative tissues.

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA (continuation)

Crop Model	Description
Biomass partitioning	
APSIM	<p>The biomass is partitioned to roots, leaves, branches, pods, grains and oil, in function of crop phase. Roots have a fixed value for each phase related with mass diverged to shoot. Between emergence and flowering, leaves and branches receive all biomass, but if leaves receive the minimum required, the remained is diverge to branches, but if the minimum is not supplied, leaf growth is penalize. Between flowering and beginning of grain filling, the leaves, pods and branches receive dry mass, and if leaves are all supply, the remained is sent to pods and branches. From beginning of grain filling to maturity, the seeds, pods and branches are supplied, with seeds demand being function of rate of increase of harvest index, potential harvest index and seed composition, while pods receive a fraction of biomass sent to the seeds. If there is over biomass after the supply to seeds and pods demand, the remained is sent to leaves and branches. The model considers a fraction from each part that can be retranslocated if daily production is not enough to supply seed growth.</p>
MONICA	<p>The model uses a matrix of distribution in function of crop phases and the part of crop that receives the biomass produced. The root growth occurs until beginning of flowering, and after that begins the addition of mass to pods (pod+seed). When the first pod is added, all biomass is diverged to pod growth until the end of the cycle.</p>
Root growth and distribution in the soil	
FAO	<p>The root depth increase in the same way than Kc curve (quadratic curve) until the moment of maximum Kc, where root depth is maximum until the maturity. It was considered that the water between wilting point and field capacity are available to the crop until the current depth of root.</p>
AQUACROP	<p>The model uses an exponential root growth function, with the maximum root depth being a function of thermal time. The current roots depth affects the water available to the crop.</p>
DSSAT	<p>The soil root growth factor (SRGF) defines how root dry mass is distributed along soil profile. The model considers root growth based on the mass diverged to root, which can be changed by water deficit. The increasing of the roots in depth is function of a potential rate per physiological day that is penalize by limiting factors, as soil water content. The root mass and the coefficient to converted mass to length are used to estimate the root density per layer.</p>

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA

(continuation)

Crop Model	Description
Root growth and distribution on the soil	
APSIM	Root growth rate is define in the model per crop phase, dry mass diverged to root, water deficit, temperature and XF coefficient. The XF coefficient can be used to penalize the potential rate of growth when limiting conditions are present in a specific soil layer, as high soil density or low pH. The root mass is converted in length using a specific root length coefficient (mm per gram). The model also considers root senescence.
MONICA	The root growth is simulated based on Pedersen et al. (2010), dry mass diverged to root follows Gerwitz and Page (1974) and root depth growth is function of thermal time. The maximum root depth and soil characteristics (texture and bulk density) affect the root growth rate per thermal day. The model also considers root diameter in function of soil depth, once root has a larger density at the top of the soil than at the bottom.
Evapotranspiration	
FAO	Potential crop evapotranspiration is estimated by multiplying the referential evapotranspiration (ET _o), estimated by Penman-Monteith approach (ALLEN et al., 1998), and the crop coefficient (K _c) defined by Martorano (2007) for soybean. The actual evapotranspiration is estimated following the limitation factor that has an exponential reduction in function of soil water content, based on the water balance developed by Thornthwaite and Mather (1955).
AQUACROP	The ET _o is an input in the model, which in this case was estimated following Penman-Monteith approach (ALLEN et al., 1998). This model estimated potential evaporation and transpiration using ET _o and values to crop (K _c) and soil (K _e) coefficients. K _e is estimated based on an approach of two stages for evaporation (RITCHIE, 1972), where in stage one K _e represents the maximum evaporation in function of solar radiation, and in the second stage K _e is estimated in function of soil water content due to water limitation. The K _c is obtained in function of crop canopy cover for the potential transpiration, but if water is limited, a new K _c value is used in function of soil water available for the crop.
DSSAT	Potential evapotranspiration is estimated, based on Penman-Monteith or Priestley-Taylor methods, which is partitioned in evaporation and transpiration. The soil evaporation is estimated following an approach of two stages (RITCHIE, 1972) and solar radiation intercepted, which defines the energy available to evaporation. The transpiration is obtained from the difference between potential evapotranspiration and soil evaporation (RITCHIE, 1998). If the water in the soil is enough to supply potential transpiration, this will be the actual transpiration; otherwise, the transpiration will be the total water available for root uptake. The root water uptake is compute based on the root density and soil water content per layer.

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA (continuation)

Crop Model	Description
Evapotranspiration	
APSIM	<p>The potential transpiration is defined based on the transpiration efficiency coefficient in function of growth stage and vapor pressure deficit, solar radiation and radiation use efficiency. When the root water uptake is not able to supply the water required by potential transpiration, the actual transpiration will be the total root water uptake and biomass production will be limited by actual transpiration or solar radiation, which is smaller. The root water uptake is based on K1 coefficient that limit the fraction of available water that can be extracted by root per day in each layer, being empirical and adjustable by soil layer in function of root density. Potential evaporation is estimated based on the adaptation of Priestley-Taylor approach, while actual evaporation is estimated following the approach of two stages of Ritchie (1972).</p>
MONICA	<p>ET_o is estimated by Penman-Monteith approach, estimating surface resistance in function of crop growth (height and leaf area index) and stomatal resistance (CO₂ and vapor pressure deficit effects). After obtaining ET_o, potential crop evapotranspiration is estimated using different values of crop coefficient (K_c) along the crop cycle. Potential soil evaporation is defined based on soil cover and soil water content, partitioning potential evapotranspiration in transpiration and evaporation. Actual evaporation is estimated considering potential evaporation, soil water content (reducing factor), vapor pressure in the soil, and maximum depth that supply water for evaporation. Transpiration is limited if root water uptake is not able to supply potential demand, and in this case, actual transpiration will be the same than total root water uptake. The root water uptake is function of root water uptake efficiency by soil layer and root length density in each soil layer.</p>
Climate and soil data required	
FAO	<p>The climate data required are mean air temperature (T), rainfall (R), solar radiation (SR), sunshine hours (n), photoperiod (N), relative humidity (RH) and wind speed (WS). For the soil is required the total soil water holding capacity for the crop between permanent wilting point (WP) and field capacity (FC).</p>
AQUACROP	<p>The climate inputs are minimum (T_n) and maximum (T_m) air temperatures, R and referential evapotranspiration (ET_o). For the soil is defined the saturation (Sat), FC and WP, soil depth (Sd) and saturated conductivity (K_{sat}), curve number (CN) from Soil Conservation Service (1972) and number of layer.</p>
DSSAT	<p>The climate data required are T_n, T_m, R, SR, minimum RH and WS. For the soil profile is required Sat, FC, WP, K_{sat}, soil bulk density (BD), organic matter content (OC), nitrogen content (NC), soil albedo (AL), CN and soil texture (silt, sand and clay content).</p>

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA
(continuation)

Crop Model	Description
Climate and soil data required	
APSIM	The climate data required are Tn, Tm, R and SR. The soil data are the same required by DSSAT.
MONICA	The climate data required are Tn, Tm, R, SR, RH and WS. It is required the soil texture to define a default soil with all data recorded.
Water dynamics at soil	
FAO	The crop water balance follows Thornthwaite and Mather (1955) approach. This approach has as inputs rainfall and/or irrigation, crop potential evapotranspiration and soil water holding capacity. As outputs, this approach provides actual soil water content, actual crop evapotranspiration, water deficit and water surplus, which corresponds to deep drainage or runoff. This model does not simulate infiltration or runoff. The soil water holding capacity is function of FC, WP and root depth.
AQUACROP	The model computes as the balance between the entrances (rainfall, irrigation and capillary rise) and the losses (crop evapotranspiration, runoff and deep percolation) of water in the effective rooting zone. The soil is divided in layers of 10 cm of depth. The water balance begins with the drainage in function of rainfall/irrigation less runoff. After, the water over field capacity is drainage and storage in the next soil layer, and successively until last layer, where the water is lost by deep percolation.
DSSAT	The model uses a common soil water sub-module for all crops that was adapted from CERES model (RITCHIE and OTTER, 1985), simulating infiltration and runoff from rainfall and irrigation, vertical drainage, unsaturated flow, soil evaporation and potential evapotranspiration. The soil water content defines transpiration/root water uptake relationship.
APSIM	The soil water module is based on water balance cascading method used by CERES (JONES and KINIRY, 1986) and PERFECT (LITTLEBOY et al., 1992) models. The processes simulated are runoff, drainage, potential evapotranspiration, soil evaporation, unsaturated flow and solute flux.
MONICA	It simulates the water flux by capacity approach (WEGEHENKEL et al., 2000), where the water over field capacity in one layer flows to next layer. The water capacity parameters are function of soil texture and affected by soil organic matter and bulk density. The model computes the balance between water entrances (rainfall, irrigation, snow and capillary rise) and losses, which are defined based on potential transpiration and evaporation.

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA

(continuation)

Crop Model	Description
FAO	<p style="text-align: center;">Indices of growth penalization</p> <p>The model uses the relationship between relative evapotranspiration and relative yield loss, defining the water deficit sensitivity index (K_y). The K_y index is adjusted for each crop phase and cultivar, with some phases being more sensitivity than others. Higher the sensitivity of the phase to water deficit higher is K_y. According to Battisti and Sentelhas (2015), flowering/grain filling has $K_y > 1$, whereas less sensitive phases, as vegetative period, has $K_y < 0.25$.</p>
AQUACROP	<p>The model penalizes leaf expansion as function of fraction of total water available, while stomatal closure, senescence and pollination index (affect harvest index) use a reference at permanent wilting point. These two relationships are used to estimate the coefficient K_s, used to penalize crop growth. The water deficit also responds by different levels of evapotranspiration, where crop is more penalize under higher than lower demand. If is the case, there is a factor related with soil fertility that penalize crop growth linearly.</p>
DSSAT	<p>The water deficit is computed based on the relationship between the total root water uptake and potential transpiration. This relationship affects linearly processes as photosynthesis, transpiration, dry mass diverged to root and crop development, while nitrogen fixation and leaf area expansion are affected when this relationship is lower than 1.5. The water deficit also increases leaf senescence. The nitrogen supply affects the balance of carbon and nitrogen, which will limit crop growth when not enough to supply the crop demand.</p>
APSIM	<p>The model has four different indices to penalize crop due to water deficit, with these indices affecting phenology and N fixation based on the fraction of water available in the soil, while photosynthesis and expansion are based on water supply and crop demand ratio. Although the model can use the same ratio to penalize crop, different levels are used, for example, N fixation begins to be reduced when the fraction of soil water is lower than 50%, whereas phenology is affected under 10%, and leaf expansion is more sensitive than photosynthesis. Nitrogen deficit affects crop growth, reducing photosynthesis and grain filling (high sensitivity), and affecting phenology (low sensitivity), where the index is estimated based on current, minimum and critical concentration of nitrogen in the tissues.</p>
MONICA	<p>The penalization occurs due to water deficit, nitrogen limitation, oxygen and heat stress. The water deficit use a simple index based on the actual and potential transpiration ratio, where penalization begins when this relation is lower than 1, value defined in the cultivar coefficients. For nitrogen, crop growth is penalized when the concentration is lower than the critical value. For oxygen, it is used to represent the reduction of water uptake when the soil is flooding, being based on the current and critical values of oxygen. The model also estimates the penalization due to heat, based on the temperature limit to the crop, reducing the number of new reproductive parts that will be add in the current day.</p>

Appendix D – Description of the main characteristics of crop simulation models: FAO, AQUACROP, DSSAT, APSIM and MONICA (conclusion)

Crop Model	Description
Nitrogen fixation	
FAO	These models do not simulated nitrogen fixation.
AQUACROP	
DSSAT	The biological fixation is the main supply of nitrogen for the soybean. The model considers the nitrogen balance in the soil from CERES model (GODWIN and JONES, 1991), with the uptake from the soil not being higher than crop demand. When nitrogen is limited, the crop designates carbohydrates to the expansion and formation of new nodules, improving nitrogen fixation. Nitrogen fixation is affect by temperature, water deficit, soil aeration and plant reproductive age, being nodule activity a parameter from specie characteristics.
APSIM	The nitrogen fixation is function of the potential rate in each crop phase, cultivar, the above biomass and water stress index for fixation. The nitrogen fixation will supply the crop based on the parameter that defines the preference by species for diffusion or fixation, with soybean using preferential nitrogen from diffusion than fixation.
MONICA	Crop parameters define the rate of nitrogen fixation, with nitrogen fixed from the soil. The uptake of nitrogen from the soil is based on the potential uptake, maximum N in the plant, above biomass, nitrogen in the root, root biomass, coefficient of nitrogen distribution, and total nitrogen in the crop. The uptake considers root length and the nitrogen is uptake in nitrate form through transpired water.
Process modified by elevated CO ₂	
FAO	It was used the curve present by REYENGA et al. (1999) and in APSIM (2015) to adjust gross biomass production for [CO ₂] level for C3 crops.
AQUACROP	The model adjusts the water use efficiency to estimate total biomass production under different [CO ₂] for C3 crops.
DSSAT	There is a coefficient to adjust the daily photosynthesis by [CO ₂], with this response following an asymptotic curve.
APSIM	Radiation use efficiency, transpiration efficiency and critical level of nitrogen at leaves are adjusted for different levels of [CO ₂]. For soybean, the transpiration efficiency and critical level of nitrogen at leaf were the same used for C3 crops in APSIM (2015).
MONICA	The model was adjusted to [CO ₂] following Mitchell et al. (1995) algorithms for maximum photosynthesis rate based on Farquhar and von Caemmerer (1982), where [CO ₂] affects crop photosynthesis, stomatal resistance and, consequently, transpiration.

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ANNEX

Annex A – Summary of climate condition during field experiments developed to collected data to calibration and validation of the soybean cultivar BRS 284 in different sites

Sites	Sowing date	TMi	Tmi	TMa	Tma	Tmed	SR	Rain	Irri	ETc	ETr	ETr/ETc
		°C				MJ m ⁻² day ⁻¹		mm				
Calibration												
PI	18/10/2013	32.1	19.2			26.0	24.2	455	0	769	590	0.77
		31.9	19.8			25.8	24.1	466	404	799	775	0.97
	14/11/2013	31.8	19.7	37.1	15.4	25.7	23.7	388	0	672	510	0.76
		31.8	19.7			25.6	23.6	431	417	714	679	0.95
	08/01/2014	31.5	19.3			25.3	22.4	250	0	567	380	0.67
		31.5	19.3			25.3	22.4	250	282	585	567	0.97
LO	10/10/2013	29.8	19.3			24.5	20.6	380	25	721	456	0.63
		29.8	19.3			24.5	20.6	380	195	727	546	0.75
	31/10/2013	29.7	19.2	36.3	14.1	24.4	20.2	406	20	655	414	0.63
		29.6	19.3			24.4	20.0	427	218	673	501	0.74
	19/11/2013	29.8	19.3			24.5	20.5	459	0	583	334	0.57
		29.6	19.3			24.4	20.1	484	186	618	474	0.77
FW	01/10/2013	29.5	18.0			23.7	23.0	763	10	767	736	0.96
	18/10/2013	30.1	18.3			24.2	23.3	808	0	739	714	0.97
	08/11/2013	30.4	18.8	36.7	6.6	24.5	23.2	762	0	682	647	0.95
	25/11/2013	30.1	18.8			24.4	22.3	761	0	650	570	0.88
	15/12/2013	30.1	18.8			24.4	21.9	759	10	635	551	0.87
	Validation											
PI	29/11/2014	30.4	19.7			25.1	20.5	773	0	415	403	0.97
	08/12/2014	30.4	19.6	37	14.8	24.9	20.6	759	0	420	403	0.96
	22/12/2014	30.7	19.8			25.2	21.1	759	0	422	389	0.92
FW	21/10/2014	29.7	19.3			24.5	21.0	435	0	318	317	1.00
	19/11/2014	29.7	19.2	34.5	13.3	24.3	21.1	439	0	381	369	0.97
	18/12/2014	29.7	19.1			24.4	21.1	533	0	422	360	0.85
AJ	29/10/2013	30.9	18.7	36.3	12.9	24.7	22.0	676	0	650	574	0.88
DO	19/10/2013	32.6	20.3			26.4	22.4	509	0	602	485	0.81
	31/10/2013	32.4	20.3	37.9	14.5	26.3	21.8	632	0	657	526	0.80
	26/09/2013	32.9	20.4			26.6	22.7	628	0	642	616	0.96
MA	11/10/2013	33.0	20.3	37.6	15.6	26.6	23.0	714	0	660	610	0.92
	21/10/2013	32.9	20.4			26.6	22.6	706	0	664	569	0.86
NA	09/10/2013	33.1	21.7			27.4	22.7	443	0	638	572	0.90
	18/10/2013	33.3	21.8	38.7	17.4	27.5	22.6	476	0	698	581	0.83
SG	14/10/2013	30.6	19.6			25.0	22.7	567	0	569	537	0.94
	25/10/2013	30.6	19.7	34.3	16.4	25.1	22.3	636	0	631	576	0.91

PI= Piracicaba, SP; LO= Londrina, PR; FW= Frederico Westphalen, RS; AJ= Antônio João, MS; DO= Dourados, MS; MA= Maracaju, MS; NA= Naviraí, MS; SG= São Gabriel do Oeste, MS; TM= average of maximum air temperature; Tm= average of minimum air temperature; TMa= absolute maximum air temperature; Tma= absolute minimum air temperature; SR= solar radiation; Irri= irrigation; ETc and ETr= potential and actual evapotranspiration, respectively, estimated by DSSAT model

Annex B – Soil characteristics obtained for each site used in the simulations

Site	Soil characteristics								
	Area around site with this type of soil	Silt	Clay	Sand	Drainage	pH	Carbon	Nitrogen	Maximum soil depth ¹
	(%)	(%)	(%)	(%)			(%)	(%)	(cm)
Chernozem									
Bagé	44	36	19	45	Deficient	6.45	1.11	0.12	90
Urugaiana	57	36	19	45	Deficient	6.45	1.11	0.12	90
Arenosols									
Encruzilhada do Sul	56	14	10	76	High	5.00	0.85	0.09	100
Alisols									
Londrina	63	9	49	42	High	5.35	0.39	0.05	170
Bento Gonçalves	56	25	66	9	High	4.90	1.61	0.76	100
Chapecó	58	22	72	6	High	5.10	2.53	0.33	70
Presidente Prudente	61	2	19	79	Moderate	6.00	0.89	0.12	170
Oxisols									
Avaré	63	11	50	39	High	4.90	1.97	0.15	200
Campos Novos	46	25	55	20	High	4.65	1.38	0.15	120
Cascavel	49	15	74	11	High	5.10	2.41	0.20	240
Passo Fundo	79	18	73	9	High	4.45	1.08	0.15	530
Iraí	56	22	72	6	High	5.10	2.53	0.33	120
Cruz Alta	86	18	73	9	High	4.45	1.08	0.15	530
Ivinhema	85	18	71	11	High	5.10	1.62	0.16	280
Umuarama	53	21	50	29	High	5.70	0.71	0.07	75
Dourados	98	18	71	11	High	5.10	1.62	0.16	280
São Carlos	77	7	31	62	High	5.30	0.90	0.10	140
Pato Branco	52	16	80	4	High	5.40	2.31	0.13	90
Campo Mourão	42	17	76	7	High	5.40	2.83	0.25	120
Nova Cantu	54	15	74	11	High	5.10	2.41	0.20	240
Joaquim Tavorá	51	1	15	84	High	4.45	0.31	0.03	200
São Luiz Gonzaga	58	40	50	10	High	5.90	2.11	0.25	40
Cambisols									
Lages	47	34	59	7	High	4.75	2.78	0.21	150
Bom Jesus	53	26	58	16	High	4.90	2.32	0.23	180
Curitiba	40	30	27	43	High	5.50	0.99	0.11	60
Acrisols									
Indaial	50	8	41	51	High	4.95	1.69	0.14	150
Piracicaba	60	15	41	44	Moderate	5.30	1.10	0.10	75
Ponta Grossa	36	12	68	20	High	5.05	1.67	0.14	170
Irati	45	12	68	20	High	5.05	1.67	0.14	170
Santa Maria	47	43	37	20	High	5.15	0.84	0.10	150

¹In the model the maximum soil depth used were between 100 and 150 cm, adapting these values for each place together with soil root growth factor

Annex C – Main modeling approaches used by the five crop simulation models used in this study for soybean crop

Process	FAO	AQUACROP	DSSAT	APSIM	MONICA
Crop Phenology ¹	D	f(T)	f(T, DL, O)	f(T, DL)	f(T, DL)
Light Utilization ²	RUE	WUE	LP	RUE/WUE	RUE
Evapotranspiration ³	PM	PM	PM	PT	PM
Root Distribution ⁴	LIN	EXP	EXP	EXP	EXP
Water dynamics at soil ⁵	TH	C	C	C	C
Stresses involved ⁶	W	W, H	W, N	W, N, A	W, N, A, H
Number coeficientes calibrated	2	21	21	17	11
Proces modified by CO ₂ response ⁷	RUE	TE	RUE/TE	RUE/TE/CLN	F

¹D= days; f= function of air temperature (T), day length (DL) and others (O, water deficit/nutrient stress); ²RUE= radiation use efficiency; LP= leaf photosynthesis; WUE= water use efficiency; ³PM= Penman-Monteith; PT= Priestley-Taylor; ⁴LIN= linear; EXP= exponential; ⁵TH= Thornthwaite-Matter; C= capacity approach; ⁶W= water deficit; H= heat; N= nitrogen limitation; A= aeration deficit stress.⁷ RUE= radiation use efficiency; TE= transpiration efficiency; CLN= critical leaf N concentration; F= Farquhar model. Additional details about de crop models can be found: FAO: Battisti, R. **Épocas de semeadura da cultura da soja com base no risco climático e na rentabilidade líquida para as principais regiões produtoras do Brasil**. 2013. 261 p. Dissertação (Mestrado em Engenharia de Sistemas Agrícolas) - Escola Superior de Agricultura Luiz de Queiroz, Universidade de São Paulo, Piracicaba; AQUACROP: <http://www.fao.org/nr/water/aquacrop.html>; DSSAT: <http://dssat.net/>; APSIM: <https://www.apsim.info/>; MONICA: <http://monica.agrosystem-models.com>

Annex D – Summary of final coefficients calibrated and used for each soybean crop model based in the field results for cultivar BRS 284 with respectively description
(continued)

Trait	Description	Values
FAO		
Ky ¹	Water deficit sensitivity index	
S-V2	Sowing - Second trefoil	0.05
V2-R1	Second trefoil - Beginning of flowering	0.15
R1-R5	Beginning of flowering - Beginning of grain filling	0.4
R5-R7	Beginning of grain filling - beginning of maturity	0.75
R7-R8	Beginning of maturity - Maturity	0.1
MRD	Maximum root depth (m)	0.6
AQUACROP		
Tb	Base temperature below which crop development does not progress (°C)	10
TB	Upper temperature (°C) above which crop development no longer increases with an increase in temperature	35
Kc _{max}	Crop coefficient when canopy is complete but prior to senescence	1.15
MERoot	Maximum effective rooting depth (m)	1.1
SFR	Shape factor describing root zone expansion	20
MRWEup	Maximum root water extraction (m ³ water/m ³ soil.day) in top quarter of root zone	0.024
MRWEbo	Maximum root water extraction (m ³ water/m ³ soil.day) in bottom quarter of root zone	0.004
CDF	Crop determinacy linked with flowering	0
HIo	Reference Harvest Index (%)	45
HIinc	Possible increase (%) of HI due to water stress before flowering	4
HIvg	Coefficient describing positive impact on HI of restricted vegetative growth during yield formation	2
HIsc	Coefficient describing negative impact on HI of stomatal closure during yield formation	5
S-E	From sowing to emergence (growing degree days)	85
S-MRD	From sowing to maximum rooting depth (growing degree days)	998
S-SS	From sowing to start senescence (growing degree days)	1580
S-M	From sowing to maturity (growing degree days)	1800
S-F	From sowing to flowering (growing degree days)	570
DF	Length of the flowering stage (growing degree days)	356
CGC	Increase in canopy cover (in fraction soil cover per growing-degree day)	0.01
CDC	Decrease in canopy cover (in fraction per growing-degree day)	0.0142
GDD-BHI	Building-up of Harvest Index during yield formation (growing degree days)	1225
DSSAT		
CSDL	Critical short day length below which reproductive development progresses with no daylength effect (for short day plants) (h)	13
PPSEN	Slope of the relative response of development to photoperiod with time (positive for short day plants) (1/h)	0.369
EM-FL	Time between plant emergence and flower appearance (R1) (PTD ¹)	24.7
FL-SH	Time between first flower and first pod (R3) (PTD)	6.5
FL-SD	Time between first flower and first seed (R5) (PTD)	18.5
SD-PM	Time between first seed (R5) and physiological maturity (R7) (PTD)	30
FL-LF	Time between first flower (R1) and end of leaf expansion (PTD)	26
LFMAX	Maximum leaf photosynthesis rate at 30°C, 350 vpm CO ₂ , and high light (mg CO ₂ m ⁻² s ⁻¹)	1.12
SLAVR	Specific leaf area of cultivar under standard growth conditions (cm ² g ⁻¹)	340
SIZELF	Maximum size of full leaf (three leaflets) (cm ²)	185
XFRT	Maximum fraction of daily growth that is partitioned to seed-shell	1
WTPSD	Maximum weight per seed (g)	0.21
SFDUR	Seed filling duration for pod cohort at standard growth conditions (PTD)	23
SDPDV	Average seed per pod under standard growing conditions (no. Pod ⁻¹)	2.3
PODUR	Time required for cultivar to reach final pod load under optimal conditions (PTD)	12
THRSH	Threshing percentage, the maximum ratio of (seed/(seed+shell)) at maturity	74
SDPRO	Fraction protein in seeds (g(protein)/g(seed))	0.4
SDLIP	Fraction oil in seeds (g(oil)/g(seed))	0.2
FL-VS	Time from first flower to last leaf on main stem (photothermal days)	26
RHGHT	Relative height of this ecotype in comparison to the standard height per node defined in the species file	1

Annex D – Summary of final coefficients calibrated and used for each soybean crop model based in the field results for cultivar BRS 284 with respectively description
(conclusion)

Trait	Description	Values
DSSAT		
SRGF ²	Soil root growth factor	
	Layer 1 (0 - 5 cm)	1.00
	Layer 2 (5 - 15 cm)	1.00
	Layer 3 (15 - 30 cm)	0.42
	Layer 4 (30 - 40 cm)	0.34
	Layer 5 (40 - 50 cm)	0.23
	Layer 6 (50 - 60 cm)	0.20
	Layer 7 (60 - 70 cm)	0.18
	Layer 8 (70 - 100 cm)	0.16
	Layer 9 (100 - 125 cm)	0.04
Layer 10 (125 - 150 cm)	0.04	
APSIM ³		
y_hi_incr	Rate of harvest index increase (1/day)	0.011 - 0.011
x_hi_max_pot	Maximum harvest index potential (hours)	0 - 1
tt_emergence	Time from emergence to end of juvenile phase (°C day)	100 - 100
x_pp_end_of_juvenile	Photoperiod function for end of juvenile to floral initiation (hours)	13 - 13.5 - 14.2 - 15.5
y_tt_end_of_juvenile	Thermal time from end of juvenile to floral initiation (°C day)	100 - 140 - 210 - 320
x_pp_floral_initiation	Photoperiod function for initiation to flowering (hours)	13 - 13.5 - 14.2 - 15.5
y_tt_floral_initiation	Thermal time from initiation to flowering (°C day)	150 - 250 - 380 - 720
x_pp_flowering	Photoperiod function for flowering to start grain fill (hours)	13 - 13.5 - 14.2 - 15.5
y_tt_flowering	Thermal time from flowering to start grain fill (°C day)	350 - 480 - 630 - 1050
x_pp_start_grain_fill	Photoperiod function for grain filling period (hours)	13 - 13.5 - 14.2 - 15.5
y_tt_start_grain_fill	Thermal time from start to end of grain fill (°C day)	500 - 900 - 1550 - 2800
tt_end_grain_fill	Thermal time from end of grain fill to maturity (°C day)	20
tt_maturity	Thermal time from maturity to harvest ripe (°C day)	20
y_height	Plant height (mm)	0 - 1500
shoot_lag	Time lag before linear coleoptile growth starts (°C day)	15
shoot_rate	Growing thermal time increase with depth for coleoptile (°C day mm ⁻¹)	1.4
KL ²	Limit fraction of water available to be extract per day in each layer	
	Layer 1 (0 - 5 cm)	0.10
	Layer 2 (5 - 15 cm)	0.10
	Layer 3 (15 - 30 cm)	0.10
	Layer 4 (30 - 40 cm)	0.06
	Layer 5 (40 - 50 cm)	0.06
	Layer 6 (50 - 60 cm)	0.02
	Layer 7 (60 - 70 cm)	0.02
	Layer 8 (70 - 100 cm)	0.01
	Layer 9 (100 - 150 cm)	0.01
MONICA		
stage_temperature_sum ¹	Thermal time require to complete the phase (°C day)	
	Sowing – emergence (1)	140
	Emergence - end of juvenile (2)	50
	End of juvenile – Beginning of flowering (3)	555
	Beginning of flowering – First pod (4)	280
	First pod – last pod (5)	910
	Last pod – Harvest (6)	365
day_length_requirement ¹	Senescence (7)	25
	Limit inferior photoperiod requirement that under this value the rate is 1 (hours)	-13
base_day_lenght ¹	Limit superior photoperiod requirement that over this value rate is 0 (hours)	-15.8
crop_specific_max_rooting_depth	Maximum root depth (m)	0.75
slope	Soil declivity	0.05

¹Coefficient calibrated for each crop phase from the model; ²Value defined by soil layers; ³Values of thermal time and photoperiod are 4 points to curve for each coefficients

Annex E – Coefficients used in 1°, 2° and 3° phase for cultivar BRS 284 in DSSAT

Trait ¹	1° Phase ²	2° Phase ²	3° Phase ²		
CSDL	12.58	13	13		
PPSEN	0.311	0.369	0.369		
EM-FL	20.2	24.7	24.7		
FL-SH	9	6.5	6.5		
FL-SD	16	18.5	18.5		
SD-PM	35.6	30	30		
FL-LF	18	26	26		
LFMAX	1.03	1.03	1.12		
SLAVR	375	375	340		
SIZELF	180	180	185		
XFRT	1	1	1		
WTPSD	0.18	0.18	0.21		
SFDUR	23	23	23		
SDPDV	2.05	2.05	2.3		
PODUR	10	10	12		
THRSH	78	78	74		
SDPRO	0.4	0.4	0.4		
SDLIP	0.2	0.2	0.2		
FL-VS ³	9	9	26		
RHGHT ³	0.9	0.9	1		
SRGF	All	All	FW	PIRA	LOND
Layer 1 (0 - 5 cm)	1	1	1	1	1
Layer 2 (5 - 15 cm)	1	1	1	1	1
Layer 3 (15 - 30 cm)	0.63	0.63	0.3	0.45	0.5
Layer 4 (30 - 40 cm)	0.5	0.5	0.17	0.4	0.45
Layer 5 (40 - 50 cm)	0.41	0.41	0.1	0.3	0.3
Layer 6 (50 - 60 cm)	0.33	0.33	0.1	0.2	0.3
Layer 7 (60 - 70 cm)	0.27	0.27	0.08	0.2	0.25
Layer 8 (70 - 100 cm)	0.18	0.18	0.08	0.15	0.25
Layer 9 (100 - 125 cm)	0.08	0.08	0.02	0.05	0.06
Layer 10 (125 - 150 cm)	0.08	0.08	0.02	0.05	0.06

¹Traits are describe in Annex D; ²1° phase, without calibration, 2° phase, calibrating only crop development, 3° phase, with complete calibration

Annex F – Coefficients used in 1°, 2° and 3° phase for cultivar BRS 284 in APSIM

Trait ¹	1° Phase ²				2° Phase ²				3° Phase ²			
	³ 1	2	3	4	1	2	3	4	1	2	3	4
y_hi_incr	0.01	0.01			0.01	0.01			0.011	0.011		
x_hi_max_pot	0	1			0	1			0	1		
tt_emergence	100	100			100	100			100	100		
x_pp_end_of_juvenile	12.58	13.4	14.2	15	13	13.5	14.2	15.5	13	13.5	14.2	15.5
y_tt_end_of_juvenile	100	133	200	400	100	140	210	320	100	140	210	320
x_pp_floral_initiation	12.58	13.4	14.2	15	13	13.5	14.2	15.5	13	13.5	14.2	15.5
x_tt_floral_initiation	250	333	500	1000	150	250	380	720	150	250	380	720
x_pp_flowering	12.58	13.4	14.2	15	13	13.5	14.2	15.5	13	13.5	14.2	15.5
x_tt_flowering	278	370	555	1481	350	480	630	1050	350	480	630	1050
x_pp_start_grain_fill	12.58	13.4	14.2	15	13	13.5	14.2	15.5	13	13.5	14.2	15.5
y_tt_start_grain_fill	564	752	1128	3007	500	900	1550	2800	500	900	1550	2800
tt_end_grain_fill	20				20				20			
tt_maturity	20				20				20			
y_height	0	1200			0	1200			0	1500		
shoot_lag	10				15				15			
shoot_rate	1				1.4				1.4			
KL												
Layer 1 (0 - 5 cm)	0.08				0.08				0.1			
Layer 2 (5 - 15 cm)	0.08				0.08				0.1			
Layer 3 (15 - 30 cm)	0.06				0.06				0.1			
Layer 4 (30 - 40 cm)	0.06				0.06				0.06			
Layer 5 (40 - 50 cm)	0.06				0.06				0.06			
Layer 6 (50 - 60 cm)	0.06				0.06				0.02			
Layer 7 (60 - 70 cm)	0.04				0.04				0.02			
Layer 8 (70 - 100 cm)	0.02				0.02				0.01			
Layer 9 (100 - 150 cm)	0.01				0.01				0.01			

¹Traits are describe in Annex D; ²1° phase, without calibration, 2° phase, calibrating only crop development, 3° phase, with complete calibration; ³Point along the curve used by the model

Annex G – Coefficients used in 1°, 2° and 3° phase for cultivar BRS 284 in MONICA

Trait ¹	1° Phase ²	2° Phase ²	3° Phase ²
stage_temperature_sum ³			
Phase 1	148	140	140
Phase 2	50	50	50
Phase 3	611	555	555
Phase 4	430	280	280
Phase 5	500	910	910
Phase 6	929	365	365
Phase 7	25	25	25
day_length_requirement ³	-12.58	-13	-13
base_day_lenght ³	-15.8	-15.8	-15.8
crop_specific_max_rooting_depth	150	150	75
slope			
PIRA	0	0	0.03
FW	0	0	0.05
LOND	0	0	0.05

¹Traits are describe in Annex D; ²1° phase, without calibration, 2° phase, calibrating only crop development, 3° phase, with complete calibration; ³Used from phase 2 to 6

Annex H – Coefficients used in 1°, 2° and 3° phase for cultivar BRS 284 in AQUACROP

Trait ¹	1° Phase ²	2° Phase ²	3° Phase ²
Tb	5	10	10
TB	30	35	35
K _{Cmax}	1.1	1.1	1.15
MERoot	2	2	1.1
SFR	15	15	20
MRWEup	0.012	0.012	0.024
MRWEbo	0.003	0.003	0.004
CDF	1	1	0
Hlo	40	40	45
Hlinc	3	3	4
Hlvg	-9	-9	2
Hlsc	3	3	5
S-E	200	85	85
S-MRD	1934	998	998
S-SS	2200	1580	1580
S-M	2700	1800	1800
S-F	1500	570	570
DF	600	356	356
CGC	0.005	0.005	0.01
CDC	0.0015	0.0015	0.0142
GDD-BHI	1180	1180	1225

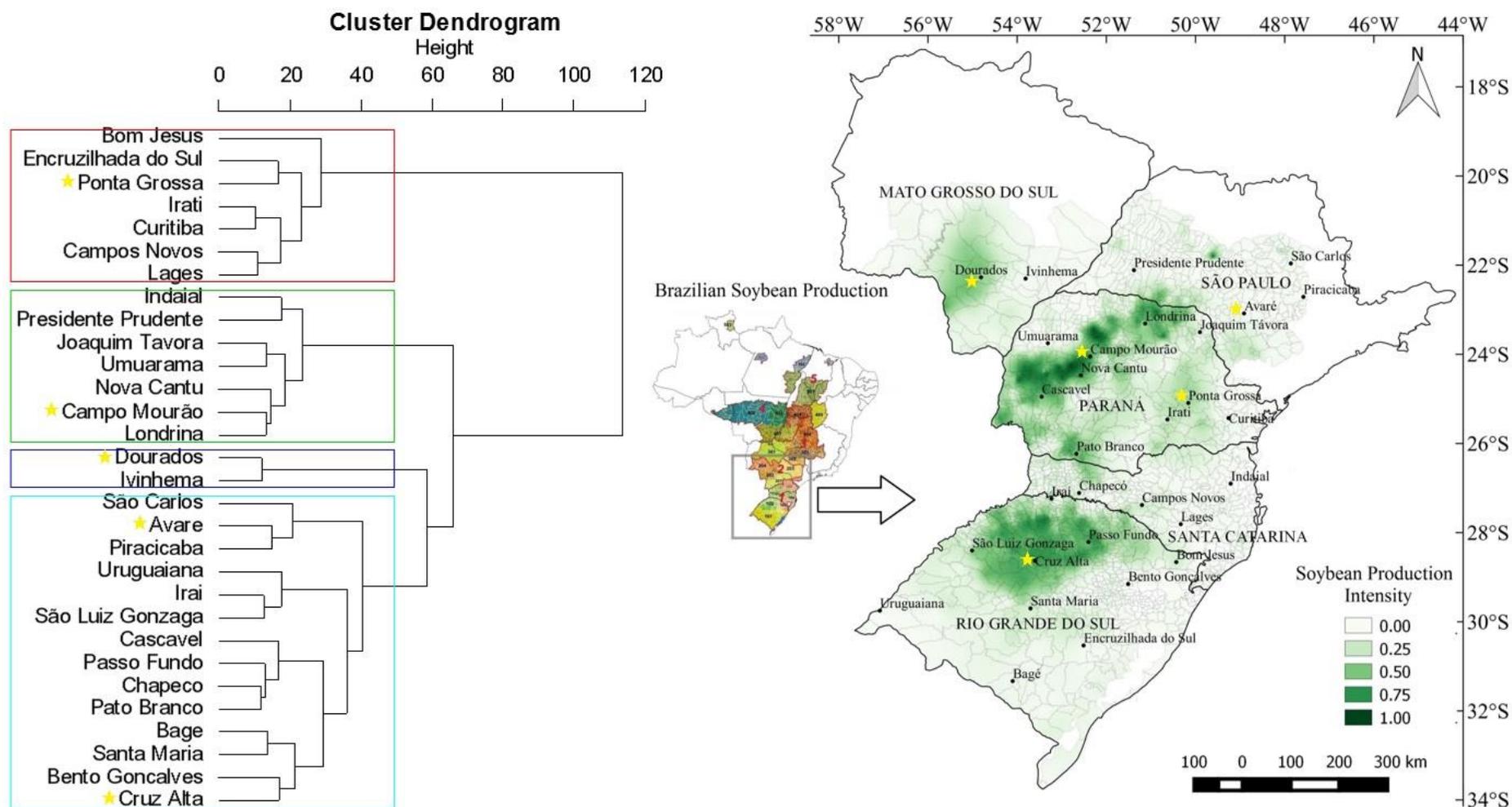
¹Traits are describe in Annex D; ²1° phase, without calibration, 2° phase, calibrating only crop development, 3° phase, with complete calibration

Annex I – Coefficients used in 1°, 2° and 3° phase for cultivar BRS 284 in FAO

Trait ¹	1° Phase ²	2° Phase ²	3° Phase ²
Ky			
S-V2	0.06	0.06	0.05
V2-R1	0.17	0.17	0.15
R1-R5			0.4
R5-R7			0.75
R7-R8			0.1
R1-R6	0.89	0.89	
R6-R8	0.08	0.08	
MRD			
Rainfed	60	60	60
Irrigated	50	50	50

¹Traits are describe in Annex D; ²1° phase, without calibration, 2° phase, calibrating only crop development, 3° phase, with complete calibration

Annex J – Geographic localization for the sites analyzed in the cluster analysis and the soybean production intensity (relative area of pixel with soybean growth), and the cluster analysis using minimum and maximum air temperature and total and standard deviation of rainfall during soybean growth. The star represents the sites selected for simulation



Annex K – Mean maximum (Max) and minimum (Min) air temperature annual and during soybean growth, solar radiation (SR) and rain during soybean growth, and air temperature delta simulated by National Institute of Space Research (INPE, 2015) for different sites in Southern Brazil, using the model ECHAM-Eta and HadCM-Eta models with Eta refined model and the HadCN3 as the border condition, based on the A1B scenario (IPCC, 2015) for mid-century (2041-2070)

Sites	Annual ¹		Soybean growth ²				Quarter ³			
	Max	Min	Max	Min	SR	Rain	DJF	MAM	JJA	SON
	°C		°C		MJ m ⁻¹ d ⁻¹	mm	°C			
Avaré	26.5	15.5	28.6	17.9	20.0	925	3.2	3.0	3.2	3.8
Bagé	23.8	13.2	28.5	17.1	19.3	673	2.4	2.4	2.6	2.2
Bento Gonçalves	22.8	13.0	26.7	16.5	20.7	728	2.4	2.4	3.0	2.6
Bom Jesus	20.8	10.5	23.9	13.6	18.5	879	2.4	2.4	3.2	2.8
Campo Mourão	27.0	14.9	29.7	18.2	17.1	873	3.2	3.2	3.4	3.6
Campos Novos	22.7	12.3	26.1	15.5	17.9	910	2.6	2.6	3.2	3.0
Cascavel	25.4	14.6	28.5	17.6	17.5	945	3.0	3.2	3.4	3.6
Chapecó	24.9	14.4	28.6	17.8	18.7	889	2.6	2.8	3.2	3.2
Cruz Alta	24.7	13.8	28.9	17.5	22.3	804	2.4	2.4	3.2	2.6
Curitiba	23.3	13.0	26.3	16.3	18.5	851	2.8	2.8	3.0	3.2
Dourados	29.2	16.8	31.7	19.9	23.4	767	3.6	3.8	3.6	4.0
Encruzilhada do Sul	22.9	13.3	27.4	16.9	16.1	635	2.4	2.4	2.6	2.4
Indaial	26.4	16.8	29.8	19.9	15.7	863	2.6	2.6	3.0	3.0
Iraí	27.4	14.6	31.5	18.5	19.5	873	2.6	2.8	3.2	3.2
Irati	23.6	12.7	26.6	16.0	18.4	823	2.8	2.8	3.2	3.4
Ivinhema	29.5	17.6	31.9	20.5	23.3	787	3.4	3.6	3.6	4.0
Joaquim Tavorá	28.1	16.0	30.7	19.3	18.9	768	3.0	3.0	3.2	3.8
Lages	21.9	11.9	25.4	15.3	16.8	798	2.4	2.4	3.2	3.0
Londrina	27.8	16.1	30.2	19.3	17.1	923	3.2	3.2	3.4	3.8
Nova Cantu	27.6	15.8	30.5	18.4	17.4	962	3.0	3.2	3.4	3.6
Passo Fundo	23.8	13.3	27.7	16.7	18.7	852	2.4	2.4	3.2	3.0
Pato Branco	25.0	14.0	28.4	17.2	18.0	941	2.8	2.8	3.4	3.4
Piracicaba	28.5	15.3	30.3	18.7	20.5	859	3.2	3.0	3.2	4.0
Ponta Grossa	24.1	13.4	27.1	16.6	15.9	837	2.8	2.8	3.2	3.4
Presidente Prudente	29.0	18.1	30.7	20.7	16.1	835	3.4	3.4	3.4	4.0
Santa Maria	25.1	14.4	29.5	18.4	19.0	767	2.4	2.4	3.0	2.4
São Carlos	26.8	15.7	28.1	18.2	20.8	1107	3.2	3.2	3.2	4.0
São Luiz Gonzaga	26.6	15.4	31.2	19.2	18.8	838	2.6	2.6	3.2	2.8
Umuarama	27.8	17.5	30.6	20.4	17.4	799	3.2	3.4	3.4	3.8
Uruguaiana	25.7	14.3	30.5	18.5	20.2	791	2.6	2.4	2.8	2.4

¹Annual average of maximum and minimum air temperature from 1961 to 2014; ²Average of maximum and minimum air temperature during soybean growth sowing at 15 Nov; ³DJF= December, January and February (summer); MAM= March, April and May (fall); JJA= June, July and August (winter); SON= September, October and November (spring). The delta is the difference between future and current climate conditions