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

Using the process-based JULES-crop model for forecasting off-season maize yield in Brazil

Amauri Cassio Prudente Junior

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

Piracicaba
2023

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versão revisada de acordo com a resolução CoPGr 6018 de 2011

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BIOGRAPHY

Amauri Cassio Prudente Junior was born in the county of Bauru-SP in 25 february of 1993, son of Amauri Cassio Prudente and Silvana Postigo Prudente. Studied the elementary school in the school São Francisco de Assis and the high school in SETA, both based in Bauru-SP. In 2011, was started Agronomic Engineering in the State University of São Paulo “Julio de Mesquita Filho” campus Ilha Solteira-SP, concluding in january of 2017. During the bachelor degree, studied one year in Spain funded by the program “Science without borders” at University of Cordoba. In march of 2017 started Master degree in the University of São Paulo, in the graduate program of Engineering of Agricultural Systems in ESALQ/USP, concluding in July of 2019. In august of 2020, he started the PhD in the same institution where submit the defense of the thesis to obtain the title of PhD in science.

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RESUMO

Utlização do modelo JULES-crop para previsão de produtividade da cultura do milho segunda safra no Brasil

A cultura do milho (*Zea mays* L.) é uma importante commodity brasileira, sendo a segunda cultura mais produzida e a quinta mais exportada no Brasil. Diante de sua relevância para diversos setores da economia, tem-se mostrado imperioso estudos que aprofundem as análises sobre as consequências dos efeitos climáticos nesta cultura, sobretudo diante de um cenário de mudanças climáticas nas próximas decadas. Para tal, modelos de culturas baseados em processos biofísicos vem sendo utilizados a fim de avaliar efeitos do clima na produtividade da cultura. No entanto, existe uma lacuna na ciência de modelos que consigam fazer simulações em larga escala devido a limitações na integração de fluxos de energia, CO_2, água e momento da atmosfera com a fisiologia da cultura. Diante disso, o modelo de superfície Joint UK land Environment Simulator (JULES), foi integrado com uma parametrização de diferentes culturas dentre as quais, o milho, porém, ainda não calibrado e avaliado no Brasil. Esta tese traz, em dois capítulos, a utilização de um modelo de larga escala na cultura do milho e a sua aplicação para prever a produção do milho safrinha no Brasil. No primeiro capítulo, objetivou-se calibrar e avaliar o modelo JULES-crop para a cultura do milho, obtendo uma alta performance para simular o indice de area foliar (IAF), altura do dossel e massa seca de grãos, tanto em condições de irrigação, quanto em sequeiro para diferentes regiões do Brasil e épocas de semeadura. No segundo capítulo, foi possível utilizar o modelo JULES-crop calibrado, além de indicadores agro-climáticos relevantes para a cultura do milho como temperatura do ar, precipitação e radiação difusa, para desenvolver um modelo de previsão de produtividade de larga escala para o milho safrinha do Brasil. A conjunção dos fatores agro-climáticos e de variáveis do modelo JULES-crop mostrou boa performance para prever a produção de milho no Brasil a partir do 80^{o} dia do ciclo. Assim, é possível afirmar que se trata de um modelo ábil para a simular em larga escala e capaz de melhorar a previsão de safra da cultura do milho no Brasil, sendo uma importante ferramenta que pode ser utilizada pela ciência para estimar a produtividade do milho em diferentes regiões produtoras brasileiras.

Palavras-chave: *Zea mays* L., JULES-crop, Mudanças climáticas, Calibração de modelos, Previsão de safra

ABSTRACT

Using the process-based JULES-crop model for forecasting off-season maize yield in Brazil

Maize (*Zea mays* L.) is an important Brazilian commodity, being the second most produced crop and the fifth most exported in Brazil. In view of its relevance for many sectors of the economy, studies that deepen the consequences of climatic effects are imperatives in face of a climate change scenario for the next decades. For this purpose, process-based biophysical models has been used to evaluate the weather effects on crop yield. However, there is a gap in the science of models able to perform in large-scale due to limitations in the integration of energy, CO_2, water and momentum fluxes with crop physiology. In view of this lacuna, the land surface model Joint UK land environment simulator (JULES) was integrated with a parametrization of different crops, among which maize, however, the model was not calibrated and evaluated in Brazil. This thesis brings in two chapters the use of a large-scale model in maize and its application to predict the off-season maize yield in Brazil. In the first chapter, the objective was to calibrate and evaluate the JULES-crop model for maize, obtaining a high performance to simulate leaf area index (LAI), canopy height and grain dry mass both for irrigated or rainfed conditions, in different regions of Brazil and sowing dates. In the second chapter, it was possible to use the calibrated JULES-crop, in addition to agro-climatic indicators such as air temperature, rainfall and diffuse radiation, to develop a large scale yield forecasting model for off-season maize in Brazil. The conjunction of agro-climatic indicators and JULES-crop outputs resulted in high performance predictions for maize yield from the 80th day of the cycle. Therefore, it is possible to confirm a skillful model to simulate in a large scale, and that it is able to improve the forecasting for maize yield in Brazil.

Keywords: *Zea mays* L., JULES-crop, Climate change, Models calibration, Yield forecasting

1. INTRODUCTION

Maize occupies a prominent place among commodities exported in Brazil, being fundamental for the worldwide food security due to its nutritive value. In Brazil, maize is the second most cultivated crop with the production of 115.2 Tg in 2021 (BRASIL, 2022), making Brazil the world's third largest producer. The high production of maize in Brazil is due to the environmental conditions allowing two growing seasons in a year: main season or first season (sown between September- December); off-season or off-season maize (sown between January-April) in succession to the soybean crop (Andrea et al., 2018; Dias et al., 2019).

Due to an imminent scenario of increase in demand for food, with projections of doubling the demand for food to attend the population in 2050 (Tilman et al., 2013), strategies to increase food production, considering the limitation for territorial expansion, are necessary for assuring the worldwide food security. Another challenging scenario for cropping systems is the climate change effects, impacting production due the rainfall irregularity and higher air temperatures as projections of IPCC (2021) indicating a minimum increase of 1.5 ^{o}C until 2040.

One of the tools used to understand weather variability and climate change impacts on crop yield is the process-based crop models (PBCM) (Rosenzweig et al., 2013). They have a set of algorythms that comprise physical and physiological aspects of the agricultural systems, being able to simulate numerically crop growth and development (Jones et al., 2017). The application of this tool for maize in Brazil has been used for different types of PBCM as DSSAT (Souza et al., 2020), Aquacrop (Silvestre et al., 2019, Souza et al., 2019) and APSIM-Maize (Santos et al., 2020). However, there is a gap in these crop models to represent CO_2, water and energy fluxes in crop growth and in large territorial areas. In view of the resolution of these deficiencies, a land surface model JULES (Joint UK Land Environment Simulator Model; Best et al., 2011, Clark et al., 2011) was adapted with a parametrization for crops generating the JULES-crop (Osborne et al., 2015). JULES-crop contain classical principes of crop phenology and carbon allocation to simulate crop growth coupled with carbon, water, energy and momentum fluxes between the surface land and atmosphere, being able to evaluate the weather and climate effects on food and water resources.

One of the applications of crop models is to forecast crop yields. The relevance to forecast crop yield at national or regional scale can potentially provide early warning for stakeholders and institutions, allowing different ways to face production decrease due to adverse climatic effects (Laudien et al., 2020). Maize has importance in the supply chain including different economic sectors such as agriculture, energy, animal feeding and marketing, and all of which would benefit from early yield forecasting. Some studies using crop models to forecast maize in different regions of Brazil were developed, however, none of these were approached in a national scale for maize using a land surface model parameterized for maize crop, incorporating CO_2, energy and water fluxes to simulate crop growth.

Due to the relevance of maize in a national scenario for economy, exploring methodologies capable to contemplate analysis in large scale using a land surface model able to integrate crop phisiology with fluxes presented in the biosphere-atmosphere process would be valuable effort for agricultural sector in a scenario of climate change in the next decades. Thus, the hypothesis of this study is that a land surface model adapted for agriculture on a large scale can contribute for reducing uncertainty for forecasting maize yield in Brazil.

1.1 Research objectives

The central objective of this thesis is to couple seasonal climate scenarios with a land surface model adapted for agriculture to forecasting maize yield in Brazil.

The specific objectives were:

1) Understand the JULES-crop growth and development parameters using a local sensitivity analysis for tropical conditions.
2) Calibrate and evaluate the JULES-crop model to simulate the maize crop in different regions of Brazil.
3) Develop and evaluate a yield forecast approach for off season maize at a national scale in Brazil using the JULES-crop model and agro-climatic indicators.

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2. CALIBRATION AND EVALUATION OF JULES-CROP FOR MAIZE IN BRAZIL

Abstract

Maize (*Zea mays* L.) is a prominent Brazilian commodity, being the second largest crop produced and fifth exported product by the country. Due to its importance for the agricultural sector, there is a concern about the effect of climate change on the crop. Process-based models are valuable tools to evaluate the effects of climate on crop yields. The Joint UK Land Environment Simulator (JULES) is a land-surface model that can be run with an integrated crop model parameterization. The resulting model (JULES-crop) thus integrates crop physiology principles with the complexity of atmosphere–biosphere coupling. It has been shown to be a valuable tool for large-scale simulations of crop yields as a function of environmental and management variables. In this study, we calibrated JULES-crop using a robust experimental dataset collected for summer and off-season maize fields across Brazil. A targeted local sensitivity analysis was performed to detect parameters of major importance during the calibration process. After calibration, the model was able to satisfactorily simulate both season and off-season cultivars. Modeling efficiency (EF) was high for leaf area index (EF =0.73 and 0.71, respectively, for summer season and off-season datasets), crop height (EF = 0.89), and grain dry mass (EF =0.61 and 0.89, respectively, for summer season and off-season datasets). The model showed a lower accuracy for simulating leaf dry mass in summer season cultivars (EF = 0.39) and soil moisture (EF = 0.44), demonstrating the necessity of further improvements including additional parametrizations of the rainfed conditions.

2.1 Introduction

Maize (*Zea mays*. L) crop has major economic and social importance in Brazil and worldwide. It is relevant for food security due to the nutritive value and chemical composition, being the third most produced crop in the world (Wijewardana et al., 2016). Brazilian maize production has been expanding over the last decades because of advances in cropping systems, positioning Brazil as the third largest world producer, with 102.5 Tg produced in 2020 (BRASIL, 2020).

Addressing the increasing demand for food, considering the limitation for territorial expansion, is one of the main agricultural challenges facing our times (Meyfroidt, 2018). FAO (2009) projects an increase in population resulting in an increase in food demand by more than 70% in 2050 in comparison to 2009. Moreover, climate change imposes other challenging aspects for maize cropping systems, such as the rainfall irregularity (Carvalho et al., 2014) and thermal stress from the higher air temperatures (Bassu et al., 2014; T. Souza et al, 2019).

Process-based crop models (PBCMs) have been a valuable tool for understanding climate change effects on crop yields (Rosenzweig et al, 2013). They contain robust physical and physiological bases organized in a set of algorithms for numerical simulations representing crop growth and development (Jones et al., 2017). Thus, PBCMs aim to simulate crop dynamics in a specific environment, considering management differences, enabling analysis with practicality and speed (Marin et al., 2014). Several PBCMs have been used to simulate maize systems in Brazil, such as Aquacrop (Silvestre et al., 2019; T. Souza et al., 2019), DSSAT-CERES-Maize (J. Souza et al., 2020; Duarte & Sentelhas, 2020), and APSIM-Maize (M. Santos et al., 2020). For studies on climate change on large territorial areas, there is a need for PBCMs that integrate crop physiology principles with biosphere–atmosphere processes.

Due to the necessity to improve the representation of crop growth and development in earth systems modelling, many studies have adjusted characteristics in land surface models to better represent the energy, CO_2, and water fluxes effects in crop growth and development in large-scale domains (Drewniak et al., 2013; Wu et al., 2016; Zhang et al., 2020). With the aim to adapt a land surface model, with the capacity to incorporate different fluxes in the biosphere–atmosphere process for crop growth simulation, a parameterization for crops was added to the land surface model Joint UK Land Environment Simulator (JULES) model (Best et al., 2011; Clark et al., 2011) by Osborne et al. (2015), which is referred to as JULES-crop. JULES-crop uses classical principles of crop phenology and C allocation to simulate crop growth coupled with C, water, energy, and momentum fluxes between the surface land and atmosphere. It also enables the assessment of weather and climate effects on food and water resources (Osborne et al., 2015). JULES-crop obtained satisfactory simulations when tested for irrigated maize in Nebraska (Williams et al., 2017). The model also performed well for rainfed maize in the North China Plain (Wolffe et al., 2021), but had mixed results when evaluated against FAO country yields (Osborne et al., 2015; Franke et al., 2020). In the study of Osborne et al. (2015), the model was not calibrated against field observations, where the parameter values were derived from the literature. Despite Osborne et al. (2015), Franke et al. (2020) presented some simulations for maize and compared with Brazilian yield recorded in FAO database, the JULES-crop had not yet been calibrated and evaluated for tropical environments as in Brazil, covering its climatic, soil, and management variability.

This paper has three major objectives: (a) to understand the JULES-crop growth and development parameters using a local sensitivity analysis for tropical conditions; (b) to calibrate the JULES-crop model using an experimental dataset conducted across the main producing regions of Brazil using the leave one-out cross validation method; and (c) to evaluate the JULES-crop predictions for different cultivars, sowing dates, and water regimes using the parameters calibrated from the cross-validation method.

2.2 Material and Methods

2.2.1 Brief model description

The model simulates crop development using a development index (DVI) varying from −2 to 2. The value −2 represents the time before the sowing, −1 represents the sowing date, 0 represents emergence, 1 represents the beginning of reproductive stage and 2 represents the end of the simulated crop season (usually harvest – see below). The DVI is used to simulate the specific leaf area (SLA), C partitioning throughout crop growth, senescence, and the harvest date. The DVI is based on the accumulation of effective temperature (T_{eff}), that is, growing degree days (Williams et al., 2017; Osborne et al., 2015), as follows in Equation 1:

$$Teff = \left\{\begin{matrix} 0 \; for \; T < Tb \\ T - Tb \; for \; Tb \le T \le To \\ (To - Tb)\left(1 - \frac{T - To}{Tm - To}\right) \; for \; To < T < Tm \\ 0 \; for \; T \ge Tm \end{matrix}\right\} \tag{1}$$

where To is optimal temperature for crop development; Tm is maximum temperature for crop development, Tb is base temperature for crop development (i.e. crop develops most rapidly when the temperature is close the optimal temperature). Each temperature adopted in this study was based in Birch et al., (1998) and Williams et al., (2017).

For crop growth simulation, the model partitions net primary productivity (NPPacc) to each plant structure and to a stem reserve pools. This partitioning is controlled by user-specified parameters. In the case of the stem, there is a partitioning for the structure and for the reserve, therefore, it also depends on a remobilization adjustment. To define the crop partitioning factors for each carbon pool (pi), the following equation was used:

$$\text{pi} = \frac{\exp(\alpha i + \beta i DVI)}{\sum_j \exp(\alpha j + \beta j DVI)} \quad (2)$$

where j= stem, leaf, harv and root. αi and βi are numerical constants that are adjusted to observational data. $\sum_j pj = 1$.

Carbon pools are initialized (to a value specified by the user: initial_carbon_io) when DVI reaches threshold (initial_c_dvi_io). In the reproductive stage, a fraction of carbon allocated in the stem is remobilized to reproductive structure as panicle and grain. A similar process occurs for the leaf, to simulate leaf senescence reducing LAI. This occurs when DVI becomes greater than the parameter controlling the senescence phase (DVIsen=0.4) (Equation 3):

$$\text{sen\_dvi} = \mu\,(DVI - DVIsen)^{\upsilon} \quad (3)$$

where: μ and ν allometric coefficients for calculation of senescence.

Similar to carbon partitioning, the SLA is calculated as a function of DVI (Equation 4):

$$SLA = \gamma\,(DVI + 0.06)^{\delta} \quad (4)$$

where the coefficients δ and γ were derived from allometric adjustments and the ratio between leaf dry mass and its carbon fraction.

The green LAI is calculated using the leaf carbon and the SLA (Equation 5):

$$LAI = \frac{C\ leaf}{fc{,}leaf}\,\text{SLA} \quad (5)$$

where C leaf is the leaf carbon pool and fc,leaf is the carbon fraction of the dry leaves.

Under normal circumstances, harvest is triggered when the DVI reaches 2, but harvest can be triggered earlier in some circumstances (such as low soil temperatures, extreme LAI values, low plant carbon, very slow crop development; please see Williams et al., 2017 for a more detailed description). In the present study, none of our simulations triggered the early harvest procedure.

The Cstem pool is used to calculate the crop height (h) (Equation 6):

$$h = k\left(\frac{Cstem}{fc{,}stem}\right)^{\lambda} \quad (6)$$

where k and λ are allometric parameters, and the fc stem is the carbon fraction in dry stem including reserve.

2.2.2 Database description

This study used a database with seven experiments conducted across Brazil. Four of those field experiments were conducted at the College of Agriculture "Luiz de Queiroz" of the University of São Paulo, located in Piracicaba, Sao Paulo State, Brazil (Southeast region, latitude 22^{o}42'30" S, longitude 47^{o}38'30 W and altitude 546 m a.m.s.l.). Of these four experiments, two was carried out for this study and the other 2 were carried out by Souza et al., (2019). The remaining three experiments were conducted in: a) the environmental and agricultural center of the University of Maranhão, located in Chapadinha, State of Maranhão (Northeast, 43 ^{o}21'33''S, longitude 3^{o}44',26'' W and altitude 93 m a.m.s.l); b) The research and extension unit of State University of São Paulo, located in Selviria, State of Mato Grosso do Sul (Midwest region, 20^{o}22'11''S, longitude 51 ^{o}25'9'' W and altitude 345 m a.m.s.l); and c) the agronomic experimental station of University of Rio Grande do Sul, located in Eldorado do Sul, State of Rio Grande do Sul (South region, latitude 30^{o}5'9''S, longitude 51^{o}37'5'' W and altitude 18 m a.m.s.l).

The climate in Piracicaba is classified by Koppen (Alvares et al., 2013) as Cwa; in Selviria and Chapadinha, the climate classification is Aw and in Eldorado do Sul, the climate classification is Cfa. All experiments received N, P, and K fertilization recommended by Raij et al., (1996) and regular weed control. Sowing and harvest dates as well as other details on the experiments are available in Table 2.1.

Table 2.1. Description of the experimental databases used for JULES-crop calibration in four different regions of Brazil.

Experiment	Region	County	Sowing and harvest dates	Cultivar, varieties or hybrid	Treatments	[γ]Temp and rainfall	Water regime	Row spacing (m)	Plant population	References
1	Southeast	Piracicaba	29 Nov 2018 and 28 Mar 2019	DKB363	Summer season	24.9 ^{o}C, 847.4 mm	Irrigated	0.45	66,000	--
2	Southeast	Piracicaba	7 May 2016 and 18 Oct 2016	P4285YH	Off-season	19.2 ^{o}C, 653.6 mm	Irrigated	0.45	66,000	Souza et al., (2019)
3	Southeast	Piracicaba	10 Jun 2016 and 19 Oct 2016	P4285YH	Off-season	19.3 ^{o}C, 374.6 mm	Rainfed	0.9	70,000	Souza et al., (2019)
4	Southeast	Piracicaba	5 Dec 2019 and 30 Mar 2020	LG36790	Summer season	24.9 ^{o}C, 771.3 mm	Rainfed	0.9	70,000	--
5	South	Eldorado do Sul	25 Oct 1995 and 6 Mar 1996	Pionner 3230	Summer season	23.5 ^{o}C, 511 mm	Irrigated	0.75	67,000	França (1999)
6	Northeast	Chapadinha	20 Feb 2015 and 04 Jun 2015	AG 1051	Summer season	26.15 ^{o}C, 897 mm	Rainfed	0.85	58,823	Santos (2016)
7	Midwest	Selviria	02 Dec 2014 and 06 Apr 2015	DKB393	Summer season	27.4 ^{o}C, 1058 mm	Rainfed	0.45	65,000	Rosa (2017)

[γ] Average air temperature and total rainfall observed in each experimental season.

In all experiments, detailed crop growth variables were monitored, including leaf dry mass, stem dry mass, grain dry mass, crop height and leaf area index (LAI), as described by Souza et al., (2019). Root dry mass were determined based on aboveground/belowground maize crop ratio, according to Vilela and Bull (1999) and Gondim et al., (2016). Soil parameters of each experiment are described in Table 2.2. In experiment 4, soil moisture data was measured using a frequency domain reflectometry (FDR) probe (Diviner 2000), calibrated for the local soil for the 0-60 cm depth (Marin et al., 2020).

Table 2.2. Soil physical parameters required by JULES-crop, with their respective definitions and units for four Brazilian regions.

Parameter	Definition	Piracicaba (Southeast)	Selviria (Midwest)	Eldorado (South)	Chapadinha (Northeast)
b	Brooks-Corey exponential for hydraulic soil characteristics (dimensionless)	17.28	7.82	9.59	5.14
hcap	Dry heat capacity (J m^{-3} k^{-1})	1.27E+06	1.26E+06	1.26E+06	1.37E+06
sm_wilt	Soil moisture at the point of permanent wilt (m^3 m^{-3})	0.28	0.18	0.217	0.11
hcon	Dry thermal conductivity (W m^{-1} k^{-1})	1.394	0.25	0.239	0.251
sm_crit	Soil moisture at the critical point (m^3 m^{-3})	0.358	0.29	0.322	0.24
satcon	Saturation hydraulic conductivity (kg m^{-2} s^{-1})	0.01	0.01	0.01	0.01
sathh	Soil matrix suction at saturation (m)	1.37	0.17	0.204	0.17
sm_sat	Soil moisture at saturation (m^3 m^{-3})	0.463	0.43	0.433	0.42
albsoil	Soil albedo (-)	0.133	0.133	0.133	0.133

Hourly meteorological data was collected by a weather station installed near to the experimental site of Piracicaba and variables recorded and their respective model codes are described in Table 2.3. For other locations, it was used the WATCH dataset based on ERA-Interim (WFDEI) reanalysis data contemplating meteorological data from 1979 to 2016 (Weedon., 2018). JULES-crop requires downward flux of longwave radiation, and diffuse radiation, which was estimated based on the methods proposed by Prata (1996). Moreover, the model required yearly averages of atmospheric CO_2 concentration, which were obtained from the National Oceanic and Atmospheric Administration (NOAA, 2020).

Table 2.3. Meteorological variables required by JULES-crop and their respective definitions and units.

Parameter	Definition
sw_down	Downward flux of short-wave radiation (W m^{-2})
lw_down	Downward flux of long-wave radiation (W m^{-2})
Precip	Rainfall (Kg $m^{-2}s^{-1}$)
T	Air temperature (^oC)
Wind	Wind speed (m s^{-1})
Pstar	Air pressure (Pa)
Q	Specific humidity (kg kg^{-1})
diff_rad	Diffuse radiation (W m^{-2})

2.2.3 Local sensitivity analysis

JULES-crop has 130 parameters in its structure used for simulating maize growth and development, mass and energy fluxes. We use a sensitivity analysis to detect the most important parameters to focus on, when calibrating JULES-crop for different cultivars in different sites across Brazil. The local sensitivity analysis followed the methods described by Wallach et al., (2018), where the reference crop parameters were those provided by Williams et al., (2017) but using specific weather and soil data (Table 2.1, 2.2 and 2.3). Then, a +/- 3% disturbance was applied to each parameter with the aim to facilitate the understanding of sensitivity parameters, and a heat map was developed based on the average absolute difference. The output variables considered in the sensitivity analysis were: LAI (croplai, m^2 m^{-2}), crop height (cropcanht, m), crop development index (cropdvi, dimensionless), in addition to the C content in leaf yield (cropleafc, kg m^{-2}), roots (croprootc, kg m^{-2}), and stem (cropstemc, kg m^{-2}), as well as the crop harvest part (cropharvc, kg m^{-2}) and net primary production (npp, kg m^{-2}), representing the crop carbon fixation capacity.

2.2.4 Calibration procedure and statistical analysis

We organized the calibration process in two steps, one being for cultivars used in the summer season (Table 2.1), and the second for off-season maize cultivars, which corresponds to the P4285YH cultivar (Table 2.1). The JULES-crop calibration procedure was based on Williams et al., (2017), where the main allometric functions of the model were adjusted to field data. Considering that a limited number of sites were available to split data for calibration and validation, the leave-one-out cross-validation method (Marin et al., 2011, Wallach et al., 2018) was used to simultaneously include all the variability of conditions and measurements in assessing the calibration performance. The leave-one-out cross-validation was applied separately for summer and off-season cultivars, because of the genetic differences between these two groups of cultivars. The procedure of the leave-one-out cross-validation had a factorial design in which each run missed one treatment each time. Consequently, five combinations were performed for summer season cultivar and two for off-season cultivar, similar to that used by Marin et al. (2011). As related in the section 2.2.3, to determine which parameters were adjusted, a targeted sensitivity analysis was performed to determine the dependency of simulated variables on changes in key parameters. After the selection of the most sensitivity parameters, the calibration procedure was based on direct adjustment in relation to observed on field experiments, using the eye fitting calibration method (Wallach et al., 2018). We did not adjust others parameters considered well-known, such as the base temperature (t_base_io), optimum temperature (t_opt_io) and others related in Table S2. JULES-crop predictions were evaluated using the following outputs: LAI, crop height, soil moisture, leaf, stem and grain dry mass. For quantifying the model performance, we compared the observed data with simulations of LAI, soil moisture, crop height, leaf, stem and grain dry mass, using the average root mean square error (RMSE) (Loague and Green, 1991), the index of agreement (d) (Willmott et al., 2012) and the Nash-Sutcliffe efficiency index (EF) (Nash-Stucliffe, 1970), as measures of goodness-of-fit (Marin et al., 2011; Wallach et al, 2018), calculating an overall statistical indexes for both groups of summer and off-season cultivars. All other model parameters were kept at the values from Williams et al., (2017).

2.3 Results and Discussion

2.3.1 JULES-crop local sensitivity analyses

Based on the targeted local sensitivity analysis, we verified that 52 parameters were sensitive to the environmental conditions observed in experiment 1 (Southeast; Table 2.1). 28 are associated with the model functionality to simulate C4 vegetation (Table S1) and 24 are associated with the specific crop parametrization of JULES-crop (Table S2), based on the output variables described in section 2.2.3: LAI, crop height, crop development index, the carbon content in leaf, stem, root, harvest part and net primary productivity. The local sensitivity analysis revealed a greater sensitivity of JULES-crop to partitioning-related parameters (alpha1_io, alpha2_io, alpha3_io, beta1_io, beta2_io, beta3_io), and to the parameter related to the crop specific leaf area (gamma_io) (Fig. 2.1). These parameters vary according to the DVI, a model variable used for calculating plant carbon pools during different crop phenological phases. Out of these parameters, alpha3_io has the strongest influence on the fraction of NPP partitioned to leaves and therefore is the strongest influence on LAI and net primary productivity variables (Fig. 2.1, Fig S1).

The fact that the leaf-related partition parameters are more sensitive than the others may be related to the difference in carbon allocation for this structure. According to Nabinger and Pontes (2002), the balance between photosynthesis and respiration generates a quantity of carbon in which part is fixed and another part is available for constituting plant biomass in the formation of roots, reserves, stems or leaves. However, the distribution of this balance in species of the Poaceae genus is uneven to meet the internal demand of the plant, with the formation of leaves mainly in vegetative stage, when more carbon will be allocated due to the need for the plant to have a leaf area to intercept solar radiation, in comparison to the carbon allocation for stem being more constant during the cycle than in the leaves. The JULES-crop algorithm for crop growth uses the LAI to calculate the canopy radiation interception, which affects the net primary productivity. Since net primary productivity affects the leaf carbon, and thus LAI (as described in Section 2.2.2), this creates a feedback loop. Hence, compared with other parameters, changes in the alpha and beta coefficients related to leaves tend to have a greater impact compared on estimating the output variables.

Two sensitive parameters in the analysis were the base and optimum temperatures (t_base_io and t_opt_io, Fig 2.1). The JULES-crop simulation is based on the DVI, i.e. the crop development calculated by an effective temperature, calculated using the base and optimum temperature (Clark et al., 2011; Osborne et al., 2015). Other crop models have also presented temperature parameters for the crop development calculation, such as CERES-Maize (Jones et al., 2003). CERES-Maize demonstrates high sensitivity to these temperature parameters, manifested in growth and development outputs, as well as grain dry mass and LAI (Bhusal et al., 2009). However, given that the base and optimum temperatures do not vary significantly in different cultivars (Birch et al., 1998) this study focused on calibrating the carbon partitioning parameters. Another sensitive parameter observed was related to initial amount of carbon in crops (Fig 2.1), as this experiment did not measure the carbon presented near emergence, the value was adopted based on Williams et al., (2017), adjusted to the value used by Osborne et al., (2015), both studies for Maize.

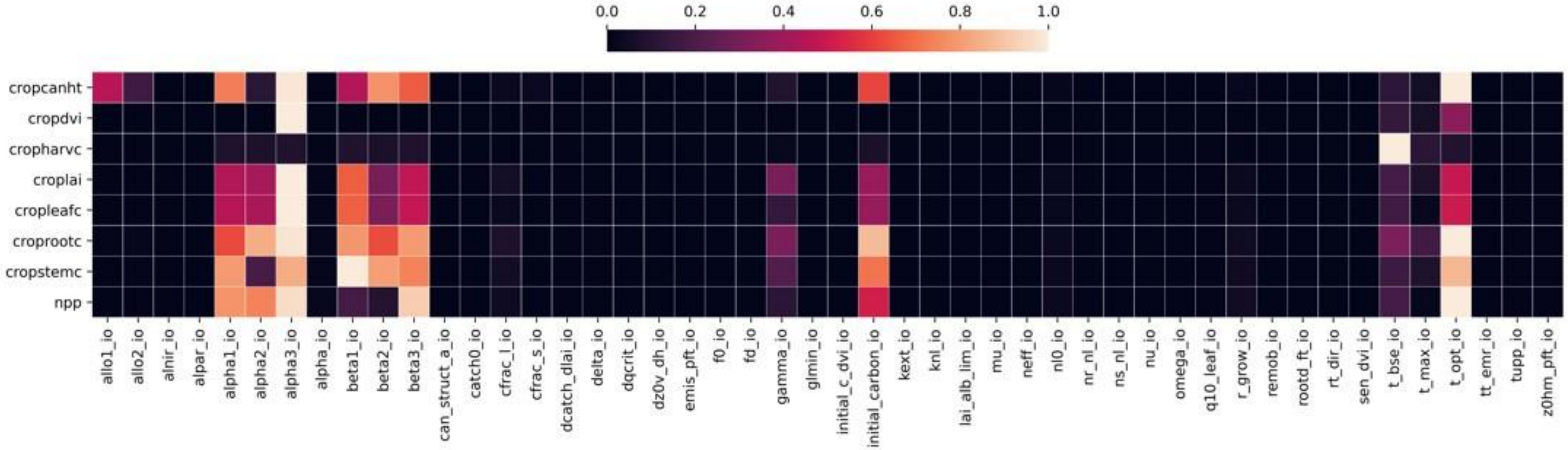

Figure 2.1. Heatmap of the local sensitivity analysis of the JULES-crop parameters for the experiment 1 (Piracicaba, SP). Greater sensitivity is expressed by values closer to 1 and clearer colors.

2.3.2 JULES-crop calibration

Compared to the parameter values reported by Williams et al., (2017) when assessing maize cultivars in Nebraska-USA, we found greater differences for cultivar P4285YH, which is commonly used for off-season crops after soybean crop in tropical producing regions of Brazil (Table 2.4). As climatic conditions in Brazil offer a wide range of viable sowing dates for maize production, there is a large availability of cultivars with distinct carbon allocation (Liang et al., 2020; Peng et al., 2020), making it necessary to calibrate off-season cultivars separately from in-season ones. Cultivars used in the summer season generally show similar patterns of growth and development, which explains the use of the same parameter values to represent this group of cultivars (Table 2.4).

The carbon partition parameters were derived using the observed data as a reference (Fig 2.2 and 2.3). In comparison to off-season cultivar, the most part of observed partitioning fractions for the summer season cultivars were shifted to higher DVI (Fig 2.2A, points, with the exception of the Pionner 3230 cultivar (South, experiment 5) when DVI between 0.5 to 1 and 1.5 to 2, so we also calibrated SLA for the two periods of crop production separately (Fig 2.2A, colored lines). Once again, this effectively mimicked the shifted pattern in DVI. The crop height measurements (Fig 2.2B) were taken only during the off-season experiment (Souza et al, 2019), so we adopted the same crop height parameters values (Table 2.4) for the summer season experiment. For the crop height parameter, the comparison used was in relation to stem dry mass as reported by Williams et al., (2017) and Osborne et al., (2015). Some patterns of carbon partitioning (Fig 2.3) and SLA (Fig 2.2A) indicate some water and thermal stress impact in grain dry mass yield (Fig 2.3D), specifically in the cultivars DKB363 (Midwest, experiment 7), AG1051 (Northeast, experiment 6) and LG36790 (Southeast, experiment 4), inducing the carbon allocation for different structures as a strategy to supply the atmospheric water demand. In the DKB363 (Midwest, experiment 7), AG1051 (Northeast, experiment 6) and LG36790 (Southeast, experiment 4), both under rainfed conditions, the flowering occurred when the air temperature exceeded the 33^{o}C, which was above the optimum temperature of 28^{o}C and influencing the carbon allocation in view of the negative impacts on the crop (Johkan et al., 2016). We verify that in experiments 6 and 7 (Northeast and Midwest) the root carbon partitioning is extended after the flowering stage (DVI>1) resulting in less carbon in the grain (Fig 2.3A and 2.3D). Such ecophysiological strategy was also observed by Pedreira et al., (2001) and Duan et al., (2019) in Poaceae species, with greater proportion of carbon allocated to the root system in relation to the above ground parts as an effect of deepening the root system towards water and nutrients. Although crop models based on fixed carbon partitioning, such as JULES-crop, can simulate the water stress in biomass gain (aboveground), it cannot simulate the effect of altered water regimes and soil nutrients on root architecture.

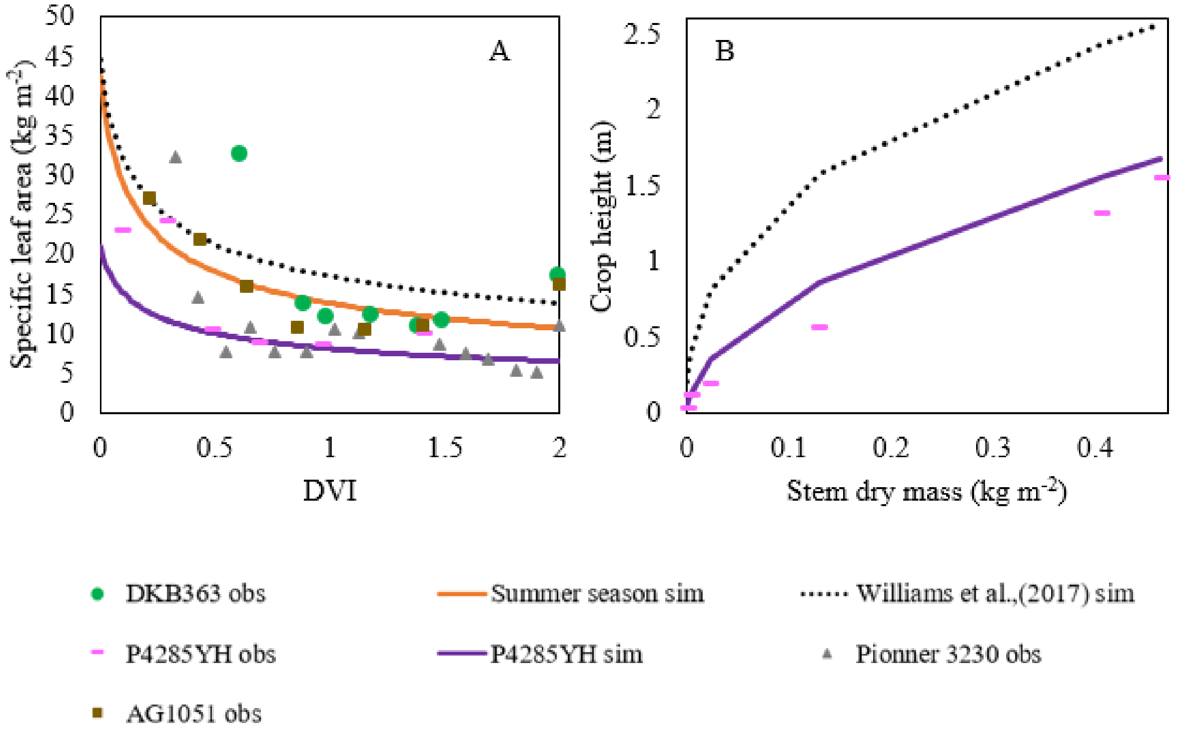

Figure 2.2. Calibrations for specific leaf area (A) and crop height (B) derived for different maize experiments conducted in four Brazilian regions. Off-season maize observations are those from cultivar P4285YH.

Table 2.4. Crop parameters adjusted for summer-season and off-season maize cultivars considered in this study in comparison with a set of parameters previously published by Williams et al., (2017).

	Williams et al., (2017)	Summer season	Off-season
α1 - root	13.5	12.2	12.2
α2 - stem	12.1	10.4	9.9
α3 – leaf	13.1	11.3	11.1
β1 - root	-15	-9.6	-9.1
β2 - stalk	-12.1	-7.4	-6.3
β3 – leaf	-14.1	-8.3	-7.8
γ (gamma_io)	17.6	14.1	14.2
δ (delta_io)	-0.33	-0.33	-0.39
λ (allo2_io)	0.38	0.52	0.52
k (allo_1_io)	3.6	2.5	2.5

We also observed a greater fraction of carbon partitioned to leaves (Fig 2.3C) in the knee-high stage of the off-season cultivar (for DVI <0.5) than in the summer season one, with a carbon partitioning around 50% allocated to leaves in the off-season cultivar in comparison to the summer cultivars, for which the carbon partitioning ranged from 30% to 45% for DKB363 (Southeast, experiment 1) and Pionner 3230 (South, experiment 5), respectively. Liang et al (2020) observed, in two maize cultivars, a decrease of carbon (C) fixation and high %C retained in leaves at low light intercepting leaves. Given that our off-season experiment reached the knee–high stage during the winter, and thus under low levels of solar radiation, we speculate that it could have been a contributing factor for a high level of carbon retained in leaves in our dataset. Yet, the leaf senescence algorithm used in JULES-crop might also be the cause of uncertainties in estimates, as our experiments did not measure the dead and live leaves along the crop cycle. The senescence algorithm was already targeted by Williams et al., (2017) in order to improve its performance, but further work is still needed.

Comparing off-season and summer season cultivars, we found difference in the stem height and mass (Fig 2.3B), these being greater in some summer cultivars than in the off-season, with carbon allocation to stems ranging from 20% to 40%, at the end of the season (DVI>1.5) in cultivars specifically in DKB363 (Southeast, experiment 1) and LG36790 (Midwest, experiment 7). However, in the tasseling stage (DVI=1) occurred the greater stem carbon allocation for off-season cultivar (Fig 2.3B), reaching 48% of the carbon distributed for the stem. Although our results contrast with off-season and Williams et al., (2017), similar carbon allocation rates at the end of season were also observed by Vasconcellos et al., (1998) in maize experiments in the southeast of Brazil using three season cultivars (BR106, AG519 and BR201). The sensitivity analysis in 3.1 summarizes the importance of modifying the carbon allocation to calibrate JULES-crop for different cultivars and sowing dates.

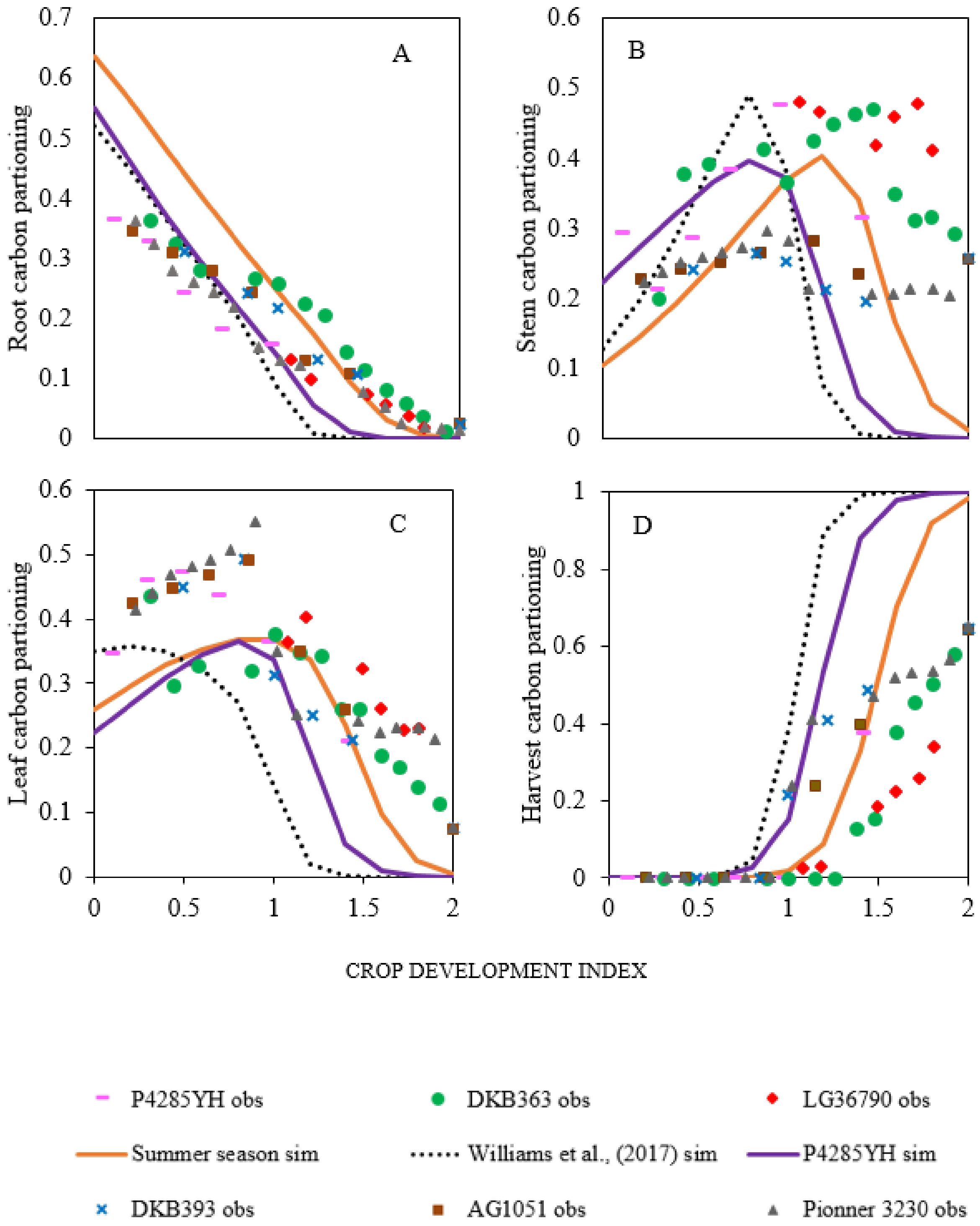

Figure 2.3. Carbon partitioning fractions for the root (A), stalk (B), leaf (C) and grain (D) carbon pools, derived for different maize experiments conducted in four Brazilian regions. Off-season maize observations use cultivar P4285YH.

2.3.3 Evaluation of the JULES-crop calibration

JULES-crop simulated maize development and growth, as well as plant structures and carbon pools during the crop cycle (Table 2.5, Fig 2.4 and 2.5) satisfactorily, in two different conditions (irrigated and rainfed) in different regions of Brazil. Using the same dataset collected for an off-season cultivar, Souza et al., (2019) calibrated the DSSAT-CERES Maize and found EF=0.70 for LAI in irrigated conditions, which is similar to this study (EF =0.71 in off-season cultivar and EF= 0.73 in summer cultivar). JULES-crop showed higher efficiency for simulating crop height in both treatments: EF=0.70 and 0.68 for irrigated and rainfed conditions found by Souza et al., (2019) in comparison to 0.88 found in this study (Table 2.5). Thus, LAI and canopy height were better simulated compared to other variables (Table 2.5, Fig 2.4 and 2.5 B, Fig 2.4 and 2.5C); moreover, it is important to highlight the grain dry mass simulation in summer cultivars (EF=0.61 for summer experiment and EF=0.89 for off-season experiment) observed in Table 2.5 and Fig 2.4D. Important to mention despite the difference between the harvest carbon partitioning for both seasons and observed data (Fig 2.3D) the model simulated grain yield with accuracy and efficiency, such as a high observation plots are along the bottom line (Table 2.5, Fig 2.3D, Fig 2.4D and 2.5D). The difference can be explained because JULES-crop remobilizes carbon from the leaf pool to the harvest pool to simulate the leaf senescence (Osborne et al., 2015; Williams et al., 2017), while the observed field data shown in Fig 2.3D are only from grain biomass gain. In general, JULES-crop presented higher levels of EF for some variables, and the model showed low efficiency in leaf dry mass and soil moisture.

Table 2.5. Statistical indexes of performances of the calibrated JULES-crop model in simulating leaf, stalk and grain dry mass, leaf area index, canopy height and soil moisture in four Brazilian regions, Brazil.

Variable	R^2	d-index	RMSE (Mg ha^{-1} m^2 m^{-2}, m or, $cm^3 cm^{-3}$)	EF
Summer season				
Stem dry mass	0.92	0.86	1.12	0.54
LAI	0.96	0.91	0.59	0.73
Leaf dry mass	0.89	0.75	1.13	0.39
Grain dry mass	0.94	0.93	1.31	0.61
Soil moisture	0.78	0.81	0.01	0.44
Off-season				
Leaf dry mass	0.89	0.71	0.46	0.63
Stem dry mass	0.93	0.91	0.98	0.71
LAI	0.95	0.98	0.34	0.71
Grain dry mass	0.96	0.94	1.03	0.89
Crop height	0.96	0.98	0.18	0.88

Soil moisture presented the second lowest value of efficiency in this study (EF=0.44 and R^2=0.78), Table 2.5). However, this is a higher value compared to the model CropSPAC, as observed by Duan et al., (2019) that demonstrate a R^2=0.78 and EF=0.26. JULES-crop also obtained a better statistical index than Santos et al., (2020b), who evaluated the APSIM-Maize model in the Brazilian northeast for simulating the soil moisture and observed RMSE ranging from 0.02 to 0.08 cm^3 cm^{-3} for several sowing times treatments, compared to the RMSE of 0.01 cm^3 cm^{-3} found in this study. Furthermore, they found an average d-index of 0.58 while this study obtained d-index=0.81. Inaccuracies for soil moisture simulations are common in crop models that utilize water balance based on texture and retention curves components, which usually overestimate simulated soil moisture, mainly because of the difficulty to estimate the surface runoff and deep drainage (Ghiberto et al., 2011). In addition, the soil moisture temporal variability of rainfed condition for DKB363 cultivar (Southeast, experiment 4), conducted under hot and wet season, was very challenging to the model as it was marked by days with heavy rainfall followed by dry spells in which moisture was severely reduced. Nonetheless, it is difficult to directly compare our results with the aforementioned studies as they do not consider the same set of observations.

Another variable that presented low efficiency was the leaf dry mass (Table 2.5, Fig 2.4F and 2.5F). This can be explained by the calibration difficulties in the senescence period. As the experiments used in this study did not separate senesced and green leaves, the alternative was to use the parameter values obtained by Williams et al., (2017). Certainly, if all experiments were standardized accounting the senesced and green leaves separation, the uncertainty of calibration would be reduced as the senescence period would be better simulated in comparison with observed data. Important to mention that cultivars LG36790 (Southeast, experiment 4), AG1051 (Northeast, experiment 6) and DKB393 (Midwest, experiment 7) were conducted under rainfed conditions, and DKB363 (Southeast, experiment 1) and Pionner 3230 (South, experiment 5) under irrigation. The rainfed cultivars showed different carbon allocation for leaves compared to irrigated scenarios as they might show distinct response in terms of leaves biomass gain rates and shortening the senescence in rainfed scenarios due to water limitations (Da Silva et al., 2012), because these type of responses are not yet captured by JULES-crop. This, in part, may be due to the use of the DVIsen value from Williams et al., (2017), which was initially derived for irrigated maize and might explain the lower EF values observed for rainfed summer maize. Another interesting aspect for the leaf dry mass low EF for summer season (Table 2.5) might be the canopy structure differences among cultivars due to the genetic diversity, in addition to the high sensitivity demonstrated in the leaf carbon partitioning and allocation in JULES-crop. One of the pieces of evidence is the higher efficiency in the off-season calibration in comparison to the summer experiments (EF=0.63 for off-season and EF=0.39 for summer calibration).

Crop models are being developed to make large-scale simulations. For example, Peng et al., (2018) combined two maize models (CLM4.5 and APSIM) with the aim to implement the maize growth simulation in a large-scale model, using a carbon allocation procedure for improving performance. The authors observed an important improvement for irrigated and rainfed treatments by joining CLM4.5 and APSIM and using databases from Nebraska (Verma et al., 2005; Suyker et al., 2004, 2005). JULES-crop could be a useful large-scale crop model with improvements such as realizing the JULES-crop calibration in different variations of nutrients as mentioned by AgMIP-GGCMI group (Elliot et al., 2015; Muller et al., 2019) given that the JULES-crop is in development.

The leave-one-out cross validation method was able to generate a calibration with high efficiency in LAI (Table 2.5, Fig 2.4 and 2.5 C), crop height (Table 2.5, Fig 2.4 and 2.5 C) and grain dry mass (Table 2.5, Fig 2.4 and 2.5 D). High efficiency in grain dry mass is important for the utilization of a large-scale crop model for crop forecasting systems in maize crop in Brazil. This method was used by Marin et al., (2011) to calibrate the few sugarcane cultivars in Brazil, posteriorly used by Marin et al., (2014) and Pagani et al., (2017). The leave-one-out cross validation method was a valuable technique for permitting the use of data not specifically collected for modeling studies, and to include both calibration and evaluation steps dealing with small datasets.

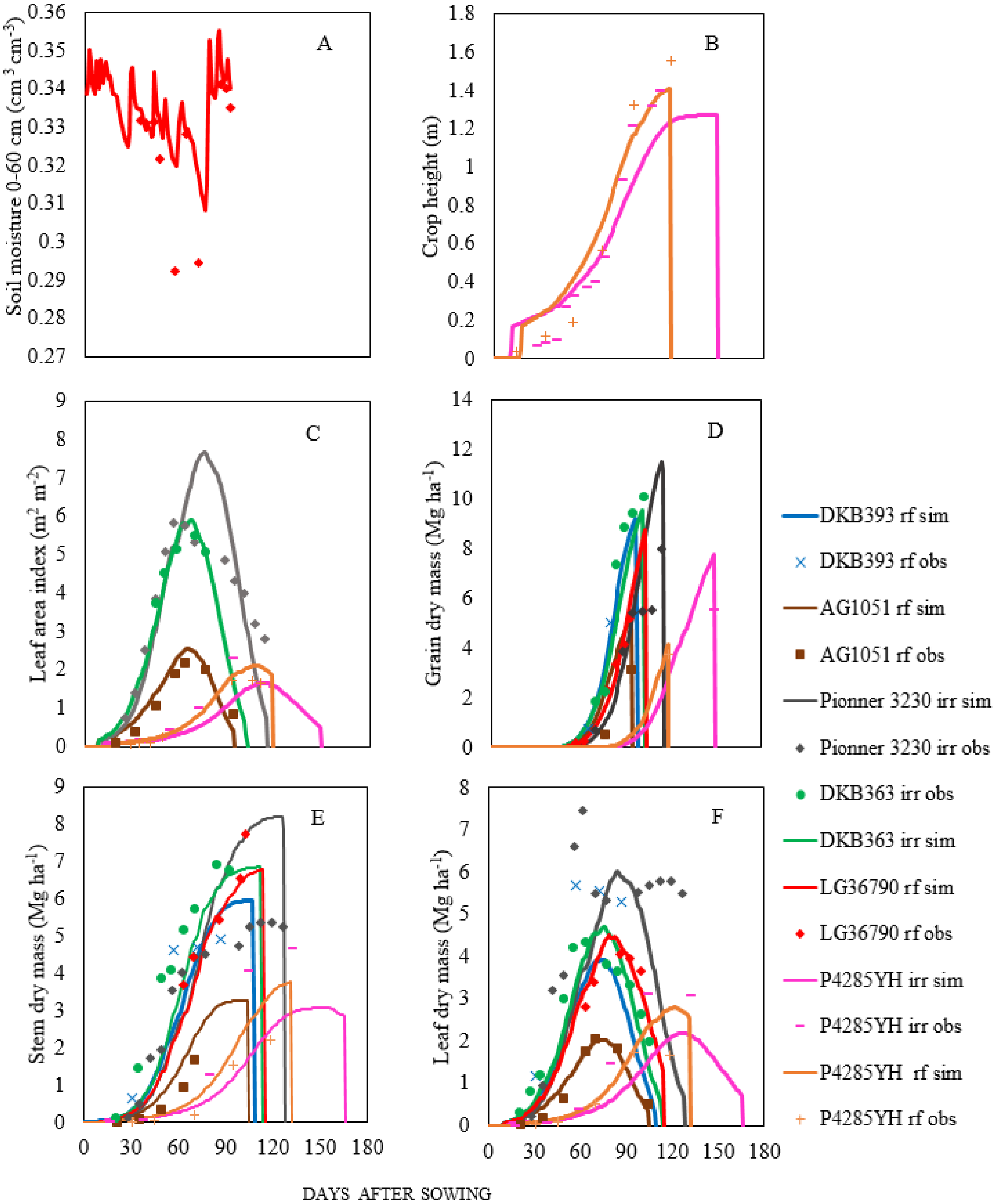

Figure 2.4. Comparison between observed and simulated variables by JULES-crop for (a) soil moisture, (b) crop height, (c) LAI, (d) grain dry mass, (e) stem dry mass, (f) leaf dry mass of different maize cultivars in different regions of Brazil. Irr-Irrigated, rf-rainfed, obs-observed, sim-simulated. Off-season maize observations use cultivar P4285YH.

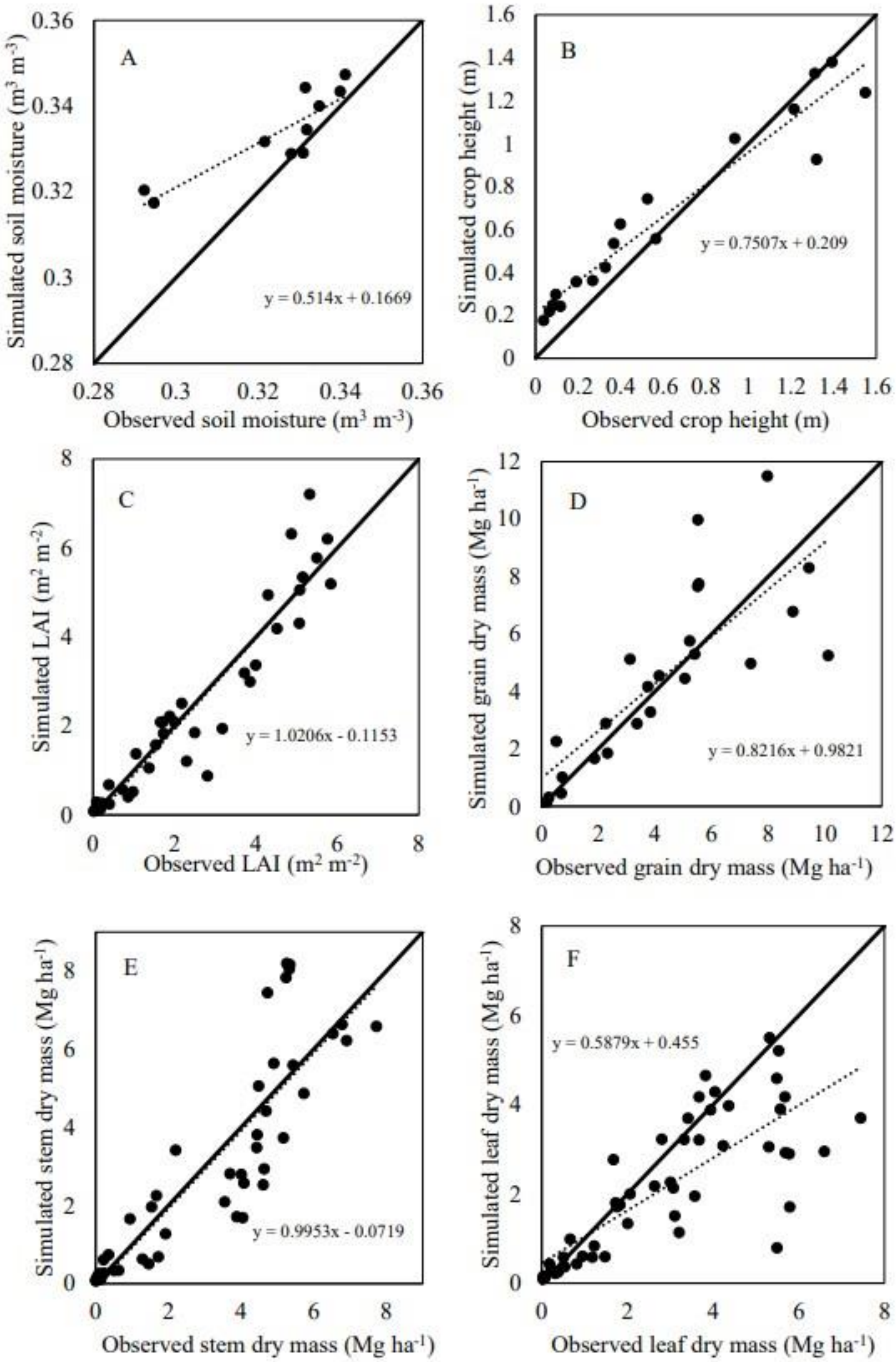

Figure 2.5: Relationship between simulated and observed values for (a) soil moisture, (b) crop height, (c) LAI, (d) grain dry mass, (e) stem dry mass, (f) leaf dry mass of maize for different regions of Brazil.

2.4 Conclusion

(i) The JULES-crop sensitivity analysis allowed us to identify which were the main parameters that should be considered during the calibration process. Mainly, they were those related to carbon partitioning and the parameters associated to the crop specific leaf area.

(ii) The JULES-crop well simulated the carbon partitioning and allometric relationships for different maize cultivars in Brazil under irrigated and rainfed regimes, for summer and off-season sowing dates.

(iii) The JULES-crop performance for simulating the development of maize crop in the field experiments was satisfactory, particularly for crop height (EF=0.89), LAI (EF=0.73 and 0.71, respectively for summer and off-season experiments) grain dry mass (EF=0.61 and EF=0.89, respectively for summer and off-season experiments). However, it demonstrated a low efficiency simulating the leaf dry mass (EF=0.39) and soil moisture (EF=0.44). The leave-one-out cross validation method was useful for calibrating different cultivar groups in different regions of Brazil with different experimental designs. The JULES-crop is a potential large-scale crop model, and its ability to evaluate climate scenarios and for forecasting maize yield in Brazil can be investigated in future studies, with improvement possibilities in fertilization rates and in rainfed scenarios.

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3 APPLICATION OF THE JULES-CROP MODEL AND AGROCLIMATIC INDICATORS FOR FORECASTING OFF-SEASON MAIZE YIELD IN BRAZIL

Abstract

Maize (*Zea mays* L.) is an important Brazilian commodity, being the second largest produced and fifth exported product by the country. In Brazil, 80 % of total production of maize is focused in the offseason (off-season) maize, mainly following the main season of soybean. Due to its relevance in the economy and food security, a maize forecasting model was developed and successfully applied in the Brazilian territory for the off-season production. The model was based on multiple linear regressions relating agroclimatic indicators and simulated outputs from JULES-crop, a land surface model applied in agriculture for large scale analysis. The resulting model was applied each 10 days after the sowing date until the maturity stage. The reliability of the forecasting model was then compared with the 2003-2016 time series of official grain yields. Agroclimatic indicators explained 60% of the inter-annual variability of maize yield in the reproductive stage. When JULES-crop outputs were added, the forecasting approach reached Nash-Sutcliffe modeling efficiency (EF) of 0.77 in the maturity stage, and EF=0.72 in the filling-grain stage, demonstrating that this method can provide useful predictions of the final maize yield from the 80th day of the cycle. JULES-crop outputs brought benefits during the vegetative stage, which decreased the standard deviation error in prediction (SDEP) from 0.59 to 0.49 Mg ha^{-1}. The overall performance indicated the yield forecasting model developed in this study was able to predict off-season maize grain yield, taking into account the challenge of climate variability in the Brazilian territory.

3.1 Introduction

Maize is an annual crop which has major importance in the worldwide economy and food security due its nutritive value (Wijewardana et al., 2016). In Brazil, maize is the second most cultivated crop with the production of 115.2 Tg in 2021 (CONAB, 2022), making Brazil the world’s third largest producer. Of the total maize production in Brazil, 88% is used as animal feed (CONAB, 2019), while the rest is used for silage (Daniel et al., 2019) and human consumption mainly in the semiarid northeast (Martins et al., 2018). Due to the Brazilian environmental conditions, maize has two growing seasons: main season or first season (sown between September-December); off-season or off-season maize (sown between January-April) in succession to the soybean crop (Andrea et al., 2018; Dias et al., 2019). Currently, off-season maize represents 80% of the total production in Brazil (CONAB, 2021), becoming thus the most important growing season for maize in the country.

Brazilian maize is relevant worldwide for food security and stands as a primary source in several supply chains, enhancing the importance of timely estimation of maize yields in Brazil. Yield forecasting at national or regional scale can potentially provide early warning for stakeholders and institutions, allowing actions before production declines due to adverse climatic effects (Laudien et al., 2020). Moreover, the maize supply chain includes different economic sectors such as agriculture, energy, marketing and animal feeding, all of which would benefit from early forecasting of yield. Early forecasting would also be useful for adjusting the food imports and regulating the agricultural markets (Basso and Liu, 2019). Furthermore, transparent yield forecasts have the function to mitigate the volatility of prices influenced by unexpected yield losses and speculative actions (OECD and FAO, 2011).

Historically, yield forecasts methods were mostly based on crop scouting and on-farm surveys (Bannayan and Crout, 1999). Such approach has however been updated in the last decades to account for crop management and weather information, by using agroclimatic indicators, remote sensing and crop modeling as basis for current yield forecasts systems (Vossen and Rijks, 1995; Bouman et al., 1997; Assad et al., 2007). Recent literature has however pointed out some deficiencies that could be improved in these forecast systems by reducing the parametrizations errors included in the model and identifying causal factors of yield fails and data uncertainties at regional scale for weather, soil properties, crop cultivars and agro-management practices (Hoffmann et al., 2016, Pagani et al., 2017).

In Brazil, maize yield forecasts were developed in different regions using distinct methods based on remote sensing data (Venancio et al., 2019), edaphoclimatic indicators (Spera et al., 2020) and crop simulation models with agroclimatic indicators (Soler et al., 2007; Martins et al., 2018; Duarte et al., 2020). Despite the relevance of these studies, none of them addressed the question of maize production in the off-season at national scale. Moreover, crop models used to develop the yield forecast in Brazil (CERES-Maize, Aquacrop and FAO-AEZ) are limited in their ability to integrate crop physiology with biosphere-atmosphere processes, not incorporating CO_2, energy and water fluxes to simulate crop growth. In view of the necessity to improve the representation of crop growth and development within Earth systems modelling, a parametrization for crops was added to the land surface Joint UK Land Environment Simulator (JULES) model (Best et al., 2011; Clark et al., 2011) by Osborne et al. (2015), which is referred to as JULES-crop. JULES-crop has obtained satisfactory simulations for maize in irrigated (Williams et al., 2017) and rainfed (Wolffe et al., 2021; Prudente Jr, 2022) conditions, however, it has not yet been used for yield forecasting at large spatial scales.

Thus, this study presents a yield forecast approach for maize based on agroclimatic indicators and on the JULES-crop model with the following objectives: (a) to identify factors that explain the maize yield variability in different phenological phases; (b) to analyze the yield forecasting model using JULES-crop outputs in potential and water limited conditions with agroclimatic indicators; and(c) to evaluate the yield forecast at national scale for maize in the off-season in Brazil.

3.2 Material and Methods

3.2.1 JULES-crop model description

The JULES-crop model simulates crop development using a development index (DVI) varying from -2 to 2. The value -2 represents the time before the sowing, -1 represents the sowing date, 0 represents emergence, 1 represents the beginning of the reproductive stage and 2 represents the end of the simulated crop season (usually harvest – see below). The DVI is used to simulate the specific leaf area (SLA), carbon partitioning throughout crop growth, senescence and the harvest date. The DVI is based on the accumulation of effective temperature (Teff), i.e. growing degree days (Williams et al., 2017; Osborne et al., 2015), as follows:

$$Teff = \left\{ \begin{matrix} 0 \; for \; T < Tb \\ T - Tb \; for \; Tb \leq T \leq To \\ (To - Tb)\left(1 - \frac{T - To}{Tm - To}\right) \; for \; To < T < Tm \\ 0 \; for \; T \geq Tm \end{matrix} \right\} \quad (1)$$

where To is optimal temperature for crop development; Tm is maximum temperature for crop development and Tb is base temperature for crop development (i.e. crop develops most rapidly when the temperature is close to the optimal temperature). Each temperature adopted for maize was based on Birch et al. (1998) and Williams et al. (2017).

For crop growth simulation, the model partitions net primary productivity (NPPacc) to each plant structure and to a stem reserve pool. This partitioning is controlled by user-specified parameters. To define the crop partitioning factors for each carbon pool (pi), the following equation was used:

$$\mathrm{pi} = \frac{\exp(\alpha i + \beta i DVI)}{\sum_j \exp(\alpha j + \beta j DVI)} \quad (2)$$

where j= stem, leaf, harvest part (grain for maize) and root. αi and βi are numerical constants that are adjusted to observational data. $\sum_j pj = 1.$ For carbon partitioned to the stem, there is a subsequent remobilization adjustment (between the structure and the reserve).

Carbon pools are initialized to a value specified by the user (initial_carbon_io) when DVI reaches threshold (initial_c_dvi_io). In the reproductive stage, a fraction of carbon allocated in the stem is remobilized to reproductive structure as panicle and grain. A similar process occurs for the leaf, to simulate leaf senescence reducing LAI. This occurs when DVI becomes greater than the parameter controlling the senescence phase (DVIsen=0.4) (Equation 3):

$$\text{sen\_dvi}= \mu\,(DVI - DVIsen)^{\upsilon} \quad (3)$$

where μ and ν are allometric coefficients for calculation of senescence.

Similar to carbon partitioning, the SLA is calculated as a function of DVI (Equation 4):

$$SLA = \gamma\,(DVI + 0.06)^{\delta} \quad (4)$$

where the coefficients δ and γ were derived from allometric adjustments and the ratio between leaf dry mass and its carbon fraction.

The green LAI is calculated using the leaf carbon and the SLA (Equation 5):

$$LAI = \frac{C\ leaf}{fc{,}leaf}\,\mathrm{SLA} \quad (5)$$

where C leaf is the leaf carbon pool and $f_{c,leaf}$ is the carbon fraction of the dry leaves.

Under normal circumstances, harvest is triggered when the DVI reaches 2, but harvest can be triggered earlier in some circumstances (such as low soil temperatures, extreme LAI values, low plant carbon, very slow crop development; please see Williams et al., 2017 for a more detailed description). In the present study, none of our simulations triggered the early harvest procedure.

The Cstem pool is used to calculate the crop height (h) (Equation 6):

$$h = k\left(\frac{Cstem}{fc{,}stem}\right)^{\lambda} \quad (6)$$

where k and λ are allometric parameters, and the $f_{c,stem}$ is the carbon fraction in dry stem including reserve.

3.2.2 Spatial distribution of maize production and model configuration

For the purpose of the study, we split Brazil into climate homogeneous zones (CZ, van Waart et al., 2013) in a total of 16 CZs (Figure 3.1) which represent 92 % of Brazilian maize production in the off-season. Simulations were run for one representative county of maize production in as reference of each CZ (Table 3.1), using hourly meteorological data obtained by the WATCH dataset based on ERA-Interim (WFDEI) re-analysis data contemplating meteorological data from 1979 to 2016 (Weedon et al., 2018). The maize growth was simulated in the most representative soil class in each CZ (greater than 10%) presented in each CZ (Table 3.1). Soil physical information of different layers (0-20 cm, 20-60 cm and 60-100 cm) was obtained by the EMBRAPA soil database (https://www.embrapa.br/solos), which were used to estimate the van Genuchten parameters for water retention curve (van Genuchten, 1980) based on pedotransfer functions of Wosten et al. (1999). JULES-crop was calibrated by Prudente Jr et al. (2022) using different maize cultivars in different sites across Brazil (Table 3.1). To analyze the maize yield for different growing regions of Brazil, it was necessary to set up the simulations according to the most typical sowing date in each CZ (Table 3.1), based on Cruz et al (2009) and Duarte and Sentelhas (2020). The harvest date was simulated by the JULES-crop model and assumed to be the same as the physiological maturity of each growing season (DVI =2.0) (Osborne et al., 2015; Williams et al., 2017).

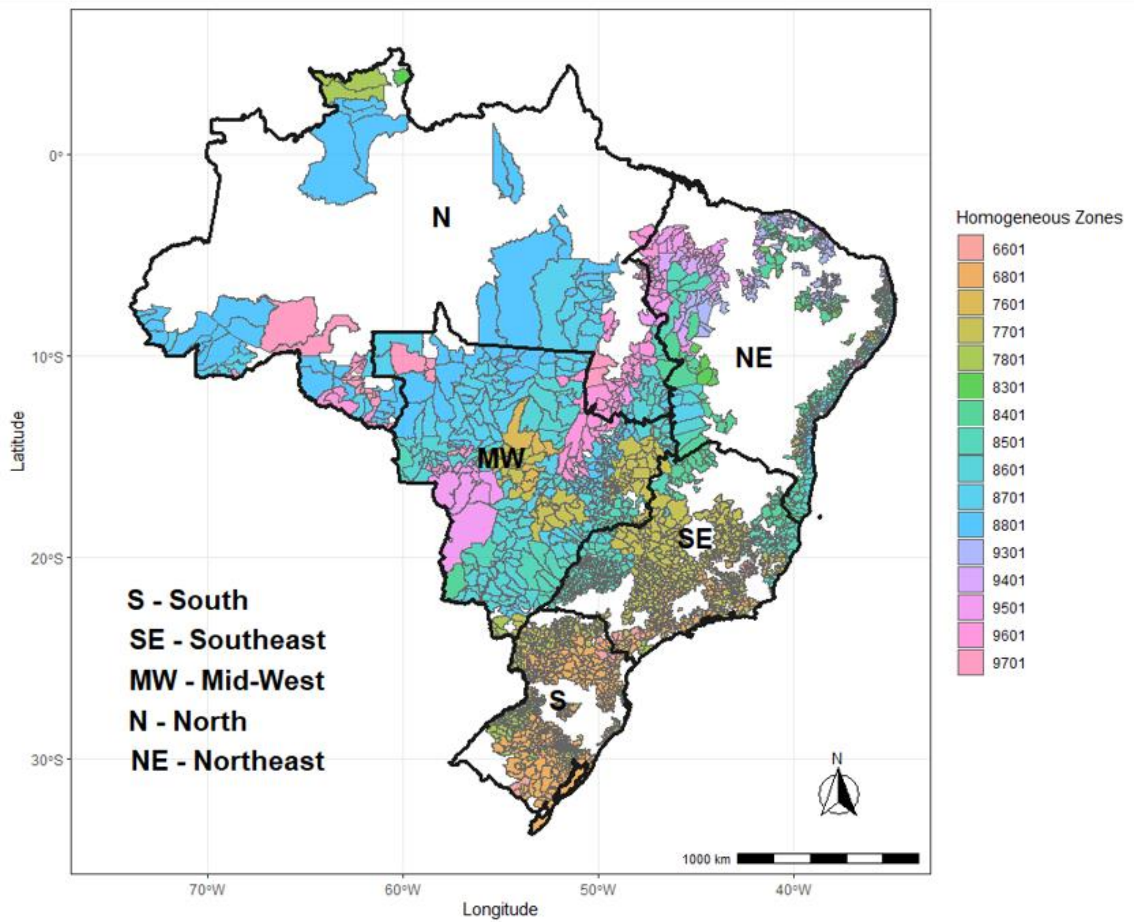

Figure 3.1. Climate homogeneous zone in the Brazilian territory used in the simulations for off-season maize yield forecast.

Table 3.1. Description of counties represented in the respective climate homogeneous zone in Brazil, used as reference to develop the maize yield forecast using the JULES-crop model outputs and agroclimatic indicators.

CZ	Latitude	Longitude	Region	County	Sowing date	Temperature and Rainfall (^{o}C and mm) $^{\gamma}$	Soil classification	(%) soil
7601	-22.037	-55.707	Midwest	Ponta Porã	1-Feb	23.14, 432	Rhodic Ferralsol	34.41
							Dystric Cambisol	16.32
6601	-23.938	-48.786	Southeast	Itapeva	1-Feb	21.27, 345	Rhodic Ferralsol	46.18
							Ferric Acrisol	32.30
8801	-12.265	-58.004	Midwest	Brasnorte	1-Feb	26.10, 604	Ferric Acrisol	58.51
							Rhodic Ferralsol	13.66
							Ferralic Arenosol	11.00
8601	-12.342	-52.533	Midwest	Querência	1-Feb	26.95,554	Rhodic Ferralsol	52.38
							Ferralic Arenosol	13.30
8701	-12.705	-55.686	Midwest	Sorriso	1-Feb	26.54,669	Rhodic Ferralsol	41.04
							Ferric Acrisol	20.06
							Ferralic Arenosol	12.67
9501	-8.224	-46.842	North	Campos Lindos	1-Feb	26.40,471	Ferric Acrisol	21.13
							Rhodic Ferralsol	16.05
							Albic Plinthosol	15.91
8401	-9.543	-46.113	Northeast	Alto Parnaíba	1-Mar	26.50,269	Dystric Leptosol	33.94
							Ferralic Arenosol	33.05
							Rhodic Ferralsol	33.01
8501	-8.495	-46.533	Northeast	Balsas	1-Mar	24.83,229	Rhodic Ferralsol	45.81
							Albic Plinthosol	14.22
							Dystric Leptosol	12.24
							Ferric Acrisol	10.70
9401	-8.280	-45.841	Northeast	Tasso Fragosso	1-Mar	26.86,267	Dystric Leptosol	36.57
							Rhodic Ferralsol	34.33
							Albic Plinthosol	16.63
9301	-8.134	-45.486	Northeast	Ribeiro Gonçalves	1-Mar	26.42,251	Rhodic Ferralsol	60.16
							Dystric	29.86

							Leptosol	
8301	-11.898	-45.411	Northeast	Barreiras	1-Apr	26.76,167	Rhodic Ferralsol	80.30
7701	-17.699	-51.015	Midwest	Rio Verde	1-Feb	24.70,414	Rhodic Ferralsol Ferralic Arenosol	40.84 22.50
7801	-24.594	-52.804	South	Campina da Lagoa	1-Feb	20.87,437	Ferric Acrisol	59.03
6801	-24.728	-53.242	South	Corbelia	1-Feb	20.68,492	Rhodic Ferralsol Dystric Leptosol Dystric Cambisol Rhodic Nitisol	41.91 17.03 15.09 10.82
9701	-13.536	-60.603	North	Cabixi	1-Apr	24.39,115	Rhodic Ferralsol Albic Plinthosol	38.80 31.60
9601	-13.108	-61.599	North	Pimenteiras do Oeste	1-Apr	25.01,127	Rhodic Ferralsol Albic Plinthosol	50.15 34.11

* Cultivar-specific parameters provided by Prudente et al. (2022)
[γ] Average air temperature and total rainfall observed during the cycle in each CZ during the period 2003-2016.

3.2.2 JULES-crop outputs and agroclimatic indicators

In order to develop the maize yield forecast model, we simulated the potential (Yp) and water limited potential yields (Yw), and calculated agroclimatic indicators for each CZ, grouped for each 10 days period of the cycle from sowing to harvest (Table 3.2). Based on Pagani et al (2017), we used two soil water balance indicators of the crop model during the cycle: FSMC (Water stress factor ranging from 0 in severe drought stress to 1 when there is no drought stress) and SWC (soil water content) from the water limited outputs simulated by JULES-crop. The SWC parameter obtained in the simulation was derived by the soil moisture minus the residual soil moisture, however, we adopted 0 for residual soil moisture due to the value in each location were not significant. For both soil parameters we considered the average from each 10 cm of depth until the effective maize root zone (60 cm). In addition, JULES-crop outputs directly related to maize yield such as the stalk dry mass (SDM), leaf dry mass (LDM), crop height (CH), leaf area index (LAI) and grain dry mass (GDM) were also included in the analysis. The agroclimatic indicators selected were: average air temperature

(TMED), diffuse incoming radiation, (DIFF_RAD) and accumulated rainfall (RAIN) from sowing to every 10-day period until the harvest (120 days) obtained in the WFDEI and in the case of diffuse radiation we based the calculus in Weiss and Norman (1985). For upscaling the forecasts at national scale, JULES-crop outputs and agroclimatic indicators were weighted according to the cultivated area of maize in the off-season in each CZ based on official statistical data provided by IBGE (IBGE, www.ibge.gov.br), for the period from 2003 to 2016. Firstly, a weighted average was calculated based on the cultivated area of off-season maize of producer counties in each CZ. After, a weighted average was calculated based on the cultivated area participation of each CZ in Brazil, generating the forecast at national scale. In each CZ, a weighted average was calculated to approach the soil percentage (Table 3.1) in the simulations of maize growth.

Table 3.2. List of JULES-crop model outputs and agroclimatic indicators selected each 10-day period and used for yield forecast.

Indicator name	Unit	Production level	Description
Model outputs			
LDM	Mg ha^{-1}	P[a], WL[b]	Leaf dry mass
SDM	Mg ha^{-1}	P, WL	Stalk dry mass
GDM	Mg ha^{-1}	P, WL	Grain dry mass
CH	M	P,WL	Crop height
LAI	m^2 m^{-2}	P,WL	Leaf area index
FSMC	0-1	WL	Integer indicating weighting of soil layers in water stress factor
SWC	m^3 m^{-3}	WL	Soil water content in the rooted zone
Agroclimatic indicator			
TMED	^{o}C	P,WL	Average daily medium temperature from sowing to the date
RAIN	mm	WL	Accumulated rainfall from sowing to the date
DIFF_RAD	MJ m^{-2} day	P,WL	Average diffuse radiation from sowing to the date

[a] Potential yield

[b] Water-limited potential yield

3.2.3 Statistical analysis

JULES-crop outputs and agroclimatic indicators (Table 3.2) were treated as independent variables for multiple linear regressions to the time series 2003-2016 of grain yield in each representative county(IBGE, www.ibge.gov.br) for each 10-days period from the sowing to the harvest (Table 3.1) depending on the sowing date considered for each CZ. A detrending procedure based on Pagani et al., (2017) was implemented, to remove the effect of significant technological trends, such as high-productive cultivars and management advances in the period. For analysis of different water management in the maize yield, the regressors were divided in three groups: JULES-crop Yp; JULES-crop Yw and agroclimatic variables. Posteriorly, a step-wise analysis was realized to identify the most suitable regressors that explained yield variability in each 10-days period from the sowing.

In order to avoid collinearity and overfitting problems in each regressor, it was calculated the Variance Inflation Factor (VIF, 1 to +∞, optimum =1) as in the following equation:

$$\text{VIF}= \frac{\mathbf{1}}{\mathbf{1}-\boldsymbol{R_i^2}} \qquad \textbf{(7)}$$

where R^2_i is the proportion of variance in the *i*th independent variable associated with the other independent variables in the model. Another factor evaluated was the presence or absence of autocorrelation among residual, for this the Durbin-Watson test was implemented (Durbin and Watson, 1971, Equation 8):

$$\text{DW}=\frac{\sum_{t=2}^{n}(e_t-e_{t-1})^2}{\sum_{t=1}^{n} e_t^2} \qquad (8)$$

where e_t is the difference between observed and predicted yield in the *t*th year of the time series; n is the number of years. Based on Savin and White (1977), the absence of autocorrelation among residuals is accepted if the result is higher than the upper critical value (dU), rejected if the result is smaller than the lower critical value (dL) and is inconclusive if the result is between dL and dU.

To evaluate the significance (p-value) of each indicator in the regression model and, with this, analyze its influence throughout the cycle, the t-test was applied. For quantifying the regression models performance, a leave-one-out cross validation (Wallach et al., 2018) was used excluding one year of forecasted yield and compared with historical yields. As measures of goodness-of-fit, based on Marin et al (2011), Pagani et al (2017) and Wallach et al (2018), was selected the cross validation-coefficient of determination (R^2) the index of agreement (d) (Willmott et al., 2012), the Nash–Sutcliffe efficiency index (EF) (Nash-Stucliffe, 1970) and the standard deviation error in prediction (SDEP, Mg ha^{-1}) to evaluate the forecast ability of different regression models.

3.3 Results

3.3.1 Statistical model selection

The stepwise analysis selected the best regression models based on JULES-crop outputs and agroclimatic indicators in each forecasting window (Table 3.3). The significance level for all the combinations of regressors was lower than 0.05 for the 80 to 120 days of the 10-day period (Table 3.3), indicating the best performance of the regressors models was in the reproductive stage of maize, in the beginning of the grain filling until maturity (days 80 to 120). The Durbin-Watson test (DW) was inconclusive to reject or accept the presence of correlation among residuals in most 10-day period; however, in the 10, 50 and 120 days after sowing, the null-hypothesis of the Durbin-Watson test was accepted (Table 3.3). Even in inconclusive cases, the null hypothesis could not be rejected. The VIF values never exceed 5.0 in each regressors model (Table 3.3), pointing out the absence of multicollinearity. In relation to the regressors model performance, the EF increased as long as there is a proximity to the maturity stage, reaching the highest values from the eightieth day to the last 10-day period (EF=0.65 and EF=0.77, respectively). The lowest values of EF was observed during the vegetative stage, in the first ten days after sowing (EF=0.43) and in the fiftieth day of the cycle (EF=0.46).

Table 3.3. Statistical indexes of performances of each forecasting window based on regressors models developed using JULES-crop outputs and agroclimatic indicators for off-season maize in Brazil.

Statistical index	Days after sowing											
	10	20	30	40	50	60	70	80	90	100	110	120
R^2	0.43	0.53	0.48	0.52	0.46	0.55	0.60	0.71	0.65	0.65	0.72	0.77
d	0.77	0.82	0.80	0.81	0.79	0.84	0.84	0.91	0.89	0.89	0.92	0.93
EF	0.43	0.53	0.48	0.52	0.46	0.55	0.60	0.71	0.65	0.65	0.72	0.77
VIF	1.75	2.13	1.92	2.08	1.85	2.22	2.50	3.45	2.86	2.86	3.57	4.35
DW	1.61	1.76	1.34	1.28	1.53	1.24	1.31	1.47	1.24	1.45	1.73	1.83
p-value	0.116	0.110	0.081	0.126	0.095	0.097	0.128	0.044	0.033	0.036	0.037	0.001

3.3.2 Selected indicators for regressors models.

A stepwise analysis allowed us to observe the factors (independent variables) influencing the grain yield (dependent variable) for each 10-day periods when compared with official yield in different CZ of Brazil. A heatmap was developed to present the most significant indicators for each regression model using maize outputs simulated for water limited conditions and agro-climatic indicators that presented better statistical performance. The most important factor observed during the maize cycle was RAIN (Figure 3.2), which was selected in all regression models by the stepwise analysis. The only exception was the first 10 days of the cycle. Another relevant agroclimatic indicator selected was TMED, being more significant in the last 10 day-period, in the maize maturity stage. Only agroclimatic indicators were responsible for explaining 60% of the maize yield variability during the days 80, 90, 110 and 120 (i.e, reproductive and maturity stage). The most frequent selected variables from JULES-crop outputs during the cycle were LAI and SDM, being significant mainly in the vegetative stage. The SWC were selected by the regression models during the tasseling stage (i.e. 80th day), which is a moment with less rainfall in the most important CZ maize producers in off-season in Brazil for CZs 8701, 7601, 7701, 6601, 8801, respectively.

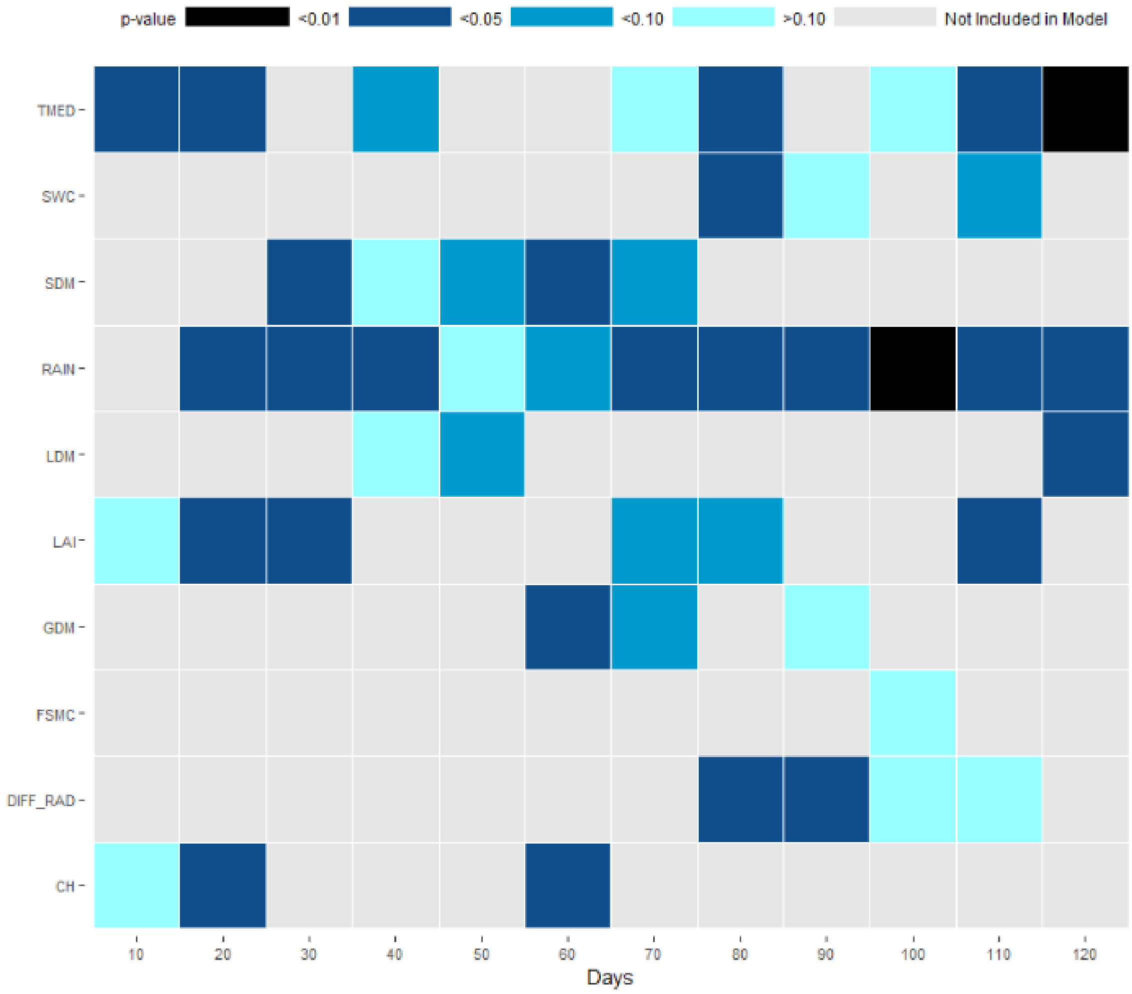

Figure 3.2: Heatmap of the indicator selected in each forecasting window based on JULES-crop outputs in water limited condition and agroclimatic indicators for maize in off-season in Brazil.

3.3.3 Yield forecast evaluation

In order to evaluate the use of JULES-crop outputs in potential and water limited conditions, it was observed the SDEP of each forecasting window and found that in none of the 10-day period, the JULES-crop potential outputs were selected by the stepwise regression, given the fact of its low statistical performance during the cycle (Figure 3.3c). In general, the agroclimatic indicators contributed to explain the inter-annual maize yield variability mainly in the reproductive stage, with SDEP varying from 0.5 to 0.38 Mg ha^{-1} (80-120 days, respectively) in the period (Figure 3.3b). However, it was observed the benefit of using JULES-crop outputs and agroclimatic indicators together in the regression models for the reproductive stage (80-120 days), reducing the SDEP by 0.4 to 0.31 Mg ha^{-1} in that stage

(Figure 3.3d). The benefits of JULES-crop water limited outputs and agroclimatic indicators were however highest during the vegetative stage (Figure 3.3d) with SDEP ranging from 0.49 to 0.46 Mg ha^{-1} while others had SDEP between 0.59 and 0.49 Mg ha^{-1} until the 70^{th} day. Furthermore, only JULES-crop outputs in water limited condition explained the grain yield variability mainly in the vegetative stage as in 30 and 50 days (SDEP =0.54 and 0.49 Mg ha^{-1}, respectively) when outputs related to leaf (LDM and LAI) and SDM prevailed (Figure 3.2, Figure 3.3a). Figure 3.4 shows the forecasted yield for maize in the off-season with the highest statistical performance in comparison with the official data. Every year, the regression models reached the official yield in any 10-day period even in the years with the highest yields in the official series (2014 and 2015). Moreover, it was possible to forecast from the 80^{th} day of the cycle near of the official data during the years of 2003-2016, being the days 80, 110, 120 those that were closest to the official yield data for maize in the off-season in Brazil (Figure 3.2, Figure 3.4).

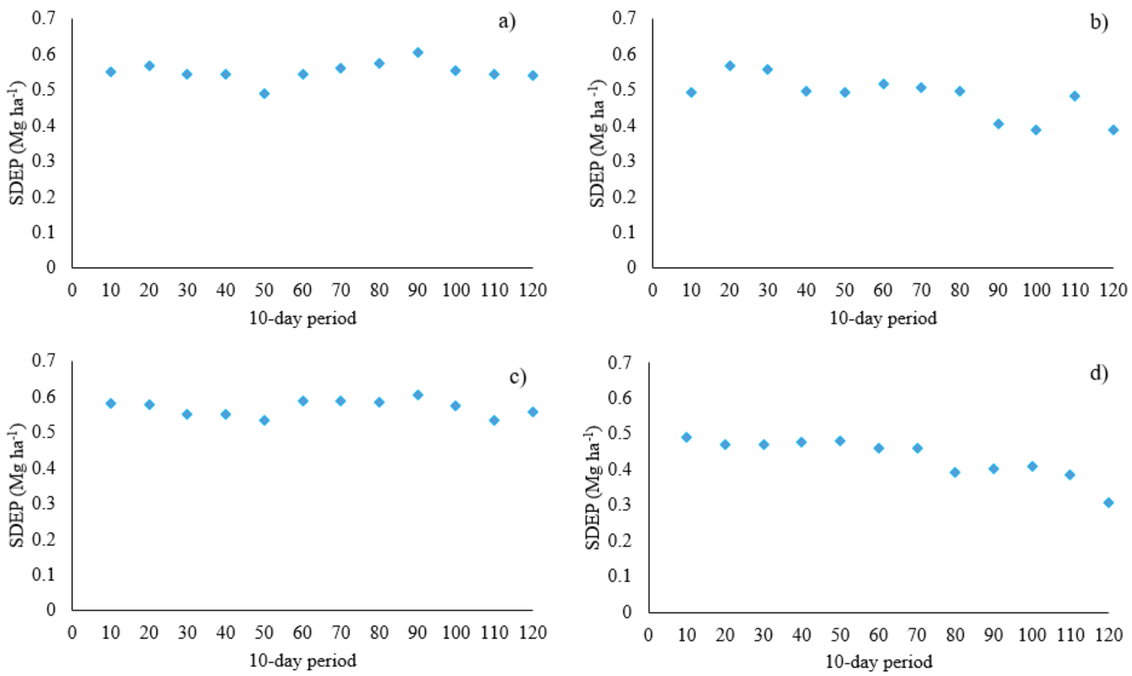

Figure 3.3. Standard deviation error in prediction (SDEP) of different forecasted yield for off-season maize in Brazil based on a) JULES-crop outputs in water limited condition; b) agroclimatic indicators; c) JULES-crop outputs in potential conditions; d) JULES-crop in water limited conditions + agroclimatic indicators.

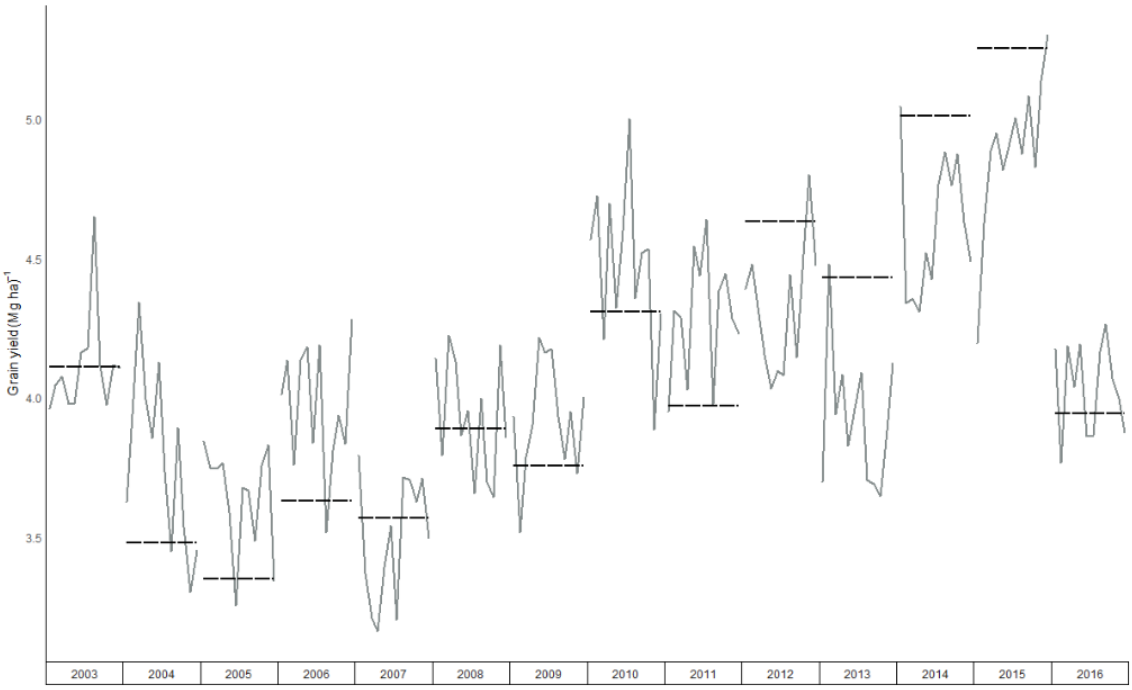

Figure 3.4. Comparison between official grain maize yield in off-season (dotted lines) and yield forecasted during the maize cycle for each day after sowing (solid line).

3.4 Discussion

The yield forecast approach for off-season maize developed in this study identified TEMP and RAIN as the main responsible for the inter-annual variability of maize yield in Brazil (Figure 3.2). Temperature influences maize biomass accumulation, interfering in the growing season length and in the average daily growth rate (Lizaso et al., 2018 and Zhu et al., 2019). Moreover, temperatures above optimum level (32^{o}C for maize) may cause failures in the pollination and injuries in the plant tissue as the metabolic activity accelerates (Johkan et al., 2011; Hatfield and Prueger 2015). Rainfall is responsible for supplying the crop water demand and maize has a high sensitivity to drought mainly during the reproductive stage, influencing the photosynthetic efficiency due to stomatal closure and wilting of leaves (Santos and Carlesso 1998 and Zhao et al., 2015). Still, the fact of the forecast approach had demonstrated two outputs related to water condition (SWC and RAIN, Figure 3.2) in the grain-filling period (around 80th day) being the most sensitive stages during the cycle (Bergamaschi et al., 2004) indicate the relevance of the water demand in the inter-annual variability in grain maize yield. The diffuse radiation was considered in this study and demonstrated significant relevance during the grain-filling period (Figure 3.2) as in Liu et al.

(2021), which observed an increase of 5.9% in yield grain under high incidence of solar radiation during grain-filling.

The integration between JULES-crop outputs and agroclimatic indices was beneficial to explain the yield variability in all forecast windows considered. Crop model and agroclimatic indices were used to develop a yield forecast system in Northeast Brazil by Martins et al. (2018) based on Aqua-crop model and weather data, reaching consistent predictions at least 30 days before harvest, similar to that found in our study. The high performance during the grain-filling (R^2=0.72) observed in this study was detected by those authors with similar precision (R^2=0.74). The same was also observed by Bussay et al. (2015) who identified a high precision to predict maize yield in Hungary during the grain-filling stages. Soler et al. (2007) used the CERES-maize model to forecast yield of off-season maize and predicted with reasonable performance around 45 days prior the harvest in Southern Brazil.

JULES-crop potential outputs were not selected by stepwise analysis in none of crop stages approached by the yield forecast model developed in this study. Pagani et al (2017) developed a sugarcane yield prediction approach for the State of São Paulo using agroclimatic indicators and DSSAT/Canegro outputs, and in none of the forecast windows considered they found the potential related variables being selected by the stepwise analysis. The authors also observed the combination of agroclimatic indicators and crop model output in water limited conditions being the best option in terms of performance for estimating the sugarcane yield. One possible reason to reject the crop outputs simulated in potential condition is the Brazilian management, characterized for rainfed crops during offseason maize, in a period where rainfall decreases near the reproductive stage in the Brazilian center-south, causing a yield gap due to the lack of water around 3.2 Mg ha^{-1} (Andrea et al., 2018).

Similar to our study, Coelho and Costa (2010) and Bergamashi et al. (2013) used a large-scale model (GLAM) for predicting maize yield in Brazil, reaching R^2=0.77 for predicting the yield in the maturity stage forecast window, similar to that we found here. Due to the fact that this study developed a maize yield forecast in a national level, large scale model outputs contributed to generate prediction with similar precision and in the same period of regional scale studies, which indicates the efficiency of the JULES-crop model to incorporate energy and water fluxes of the atmosphere in plant biomass accumulation process, explaining the high predictivity performance and jointly with temperature and precipitation being able to explain the yield variability of maize in off-season, especially during the reproductive stage.

3.5 Conclusion

This study proposed a yield forecast for maize off-season in Brazil using JULES-crop outputs and agroclimatic indicators. From a stepwise analysis, it was possible to identify regression model components in each forecast window, being precipitation and temperature mainly responsible to explain 60% of inter-annual variability of maize off-season yield in Brazil in the 2003-2016 period. Moreover, JULES-crop outputs improved the prediction ability during the reproductive stage, explaining 77% of the yield variability in the maturity stage, as well as outputs related to leaf and stem dry mass that reduced the error when together with the agroclimatic indicator during the vegetative stage. The yield forecast approach developed in this study predicted the maize yield with high performance around 40 days before the harvest (p-value<0.05) from the grain-filling stage. Finally, this study showed that JULES-crop was able to contribute to the large-scale forecast for a national approach of one of the most relevant agricultural commodities produced in Brazil.

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4 CONCLUSION AND FUTURE WORK

This Ph.D. thesis was developed in view of the necessity to improve forecasting maize yield in Brazil using a land surface model adapted for agriculture (JULES-crop) with conditions to simulate in large scale. The first step was presented in the first chapter the calibration and evaluation of JULES-crop for maize in different regions of Brazil, using a robust dataset including various cultivars, in different sesason and distincts water management. In this chapter was possible to confirm JULES-crop as a valuable tool for large-scale simulations of maize crop in Brazil, with high performance to simulate specially crop height, LAI and grain dry mass in rainfed and irrigated conditions.

In the second chapter was proposed a forecasting approach based on JULES-crop outputs and agroclimatic indicators being tested in national scale for offseason maize. The yield forecast model demonstrated high performace for predcting yield from the 80th day of the cycle, being possible to confirm the hypothesis presented in this study in which land surface model adaptaed for agriculture in large scale can contribute to reduce uncertainty to forecasting maize yield in Brazil. Another lines of investigation can be explored in the future as the utilization of whether dataset measured in meteorological stations, being more feasible to develop a forecasting system to predict maize yield. One relevant suggestion for the future is to use grid analysis (0.25^{o} x 0.25^{o}) instead climate homogeneous zone to approach the climate diversity of Brazil. Moreover, this PhD thesis can serve as a reference to demonstrate JULES-crop can be able to be used for different crops as wheat, sugarcane and soybean to predict another commodities in large scale, being a relavant tool for farmers, institutions and stakeholders to anticipate solutions for different problems can caused by extreme whether factors due to a climate change scenario in the next decades.

5 APPENDICES

Table S1. Functional parameters of JULES-crop for maize crop and its values based on Williams et al., (2017). Units of dimensionless variables are represented by (-).

Parameters	value	Definition
alpar_io	0.1	Leaf reflection coefficient for VIS (photosyntehtically active radiation) (-).
alpha_io	0.055	Quantum efficiency of photosynthesis (mol CO_2 per mol PAR photons).
can_struct_a_io	0.65	Canopy structure factor (adimensional).
catch0_io	0.5	Minimum canopy capacity (kg m^{-2}).
dcatch_dial_io	0.05	Rate of change of canopy capacity with LAI (kg m^{-2}).
dqcrit_io	0.075	Critical humidity deficit (kg H_2O per kg air).
dz0v_dh_io	0.1	Rate of change of vegetation roughness length for momentum with height (-).
emis_pft_io	1	Surface emissivity (-)
f0_io	0.4	Ratio of internal to external CO2 pressure when canopy level specific humidity deficit is zero (-).
fd_io	0.0096	Scale factor for dark respiration (-)
fsmc_p0_io	0.65	Scaling factor in water stress calculation (-)
glmin_io	1.00E-06	Minimum leaf conductance for H_2O (m s^{-1}).
infil_f_io	2	Infiltration enhancement factor (-)
kext_io	0.5	Light extinction coefficient (-)
knl_io	0	Parameter for decay of nitrogen through the canopy, as a function of LAI (-)
lai_alb_lim_io	0.5	Minimum LAI permitted in calculation of the albedo in snow-free conditions (-)
neff_io	0.00057	Scale factor relating V_{cmax} with leaf nitrogen concentration (-)
nI0_io	0.07	Top leaf nitrogen concentration (kg N (kg C) $^{-1}$).
nr_ni_io	0.195	Ratio of root nitrogen concentration to leaf nitrogen concentration (-)
ns_nl_io	0.215	Ratio of stem nitrogen concentration to leaf nitrogen concentration (-)
omega_io	0.17	Leaf scattering coefficient for PAR (-)
q10_leaf_io	1	Q10 factor for plant respiration (-)
r_grow_io	0.25	Growth respiration fraction (-)
rootd_ft_io	0.5	Parameter determining the root depth (m).
tlow_io	16	Lower temperature parameter for photosynthesis, for the Collatz model of leaf photosynthesis (^oC)
tupp_io	47	Upper temperature parameter for photosynthesis, for the Collatz model of leaf photosynthesis (^oC)
z0hm_pft_io	0.1	Ratio of the roughness length for heat to the roughness length for momentum (adimensional)

Table S2: JULES-crop parameters specific to maize crop and its values. Units of dimensionless variables are represented by (-) (Williams et al., 2017).

Parameters	value	Definition
cfrac_l_io	0.439	Carbon fraction of dry matter for leaves (-)
cfrac_s_io	0.439	Carbon fraction of dry matter for stems (-)
initial_c_dvi_io	0.1	DVI at which the crop carbon is set to initial_carbon_io (-)
initial_carbon_io	8.00E-04	Carbon in crop at emergence (kg C m^{-2}).
mu_io	0.02	Allometric coefficient for calculation of senescence (-).
nu_io	4	Allometric coefficient for calculation of senescence (-).
remob_io	0.12	Remobilisation factor (-)
rt_dir_io	0	Coefficient determining relative growth of roots vertically and horizontally (-)
sen_dvi_io	0.4	DVI at which leaf senescence begins.
t_bse_io	281.15	Base temperature (K).
t_max_io	318.15	Maximum temperature (K).
t_mort_io	273.15	Soil temperature (second level) at which to kill crop if DVI>1.
t_opt_io	303.15	Optimum temperature (K).
tt_emr_io	53.4	Thermal time between sowing and emergence (deg Cd).

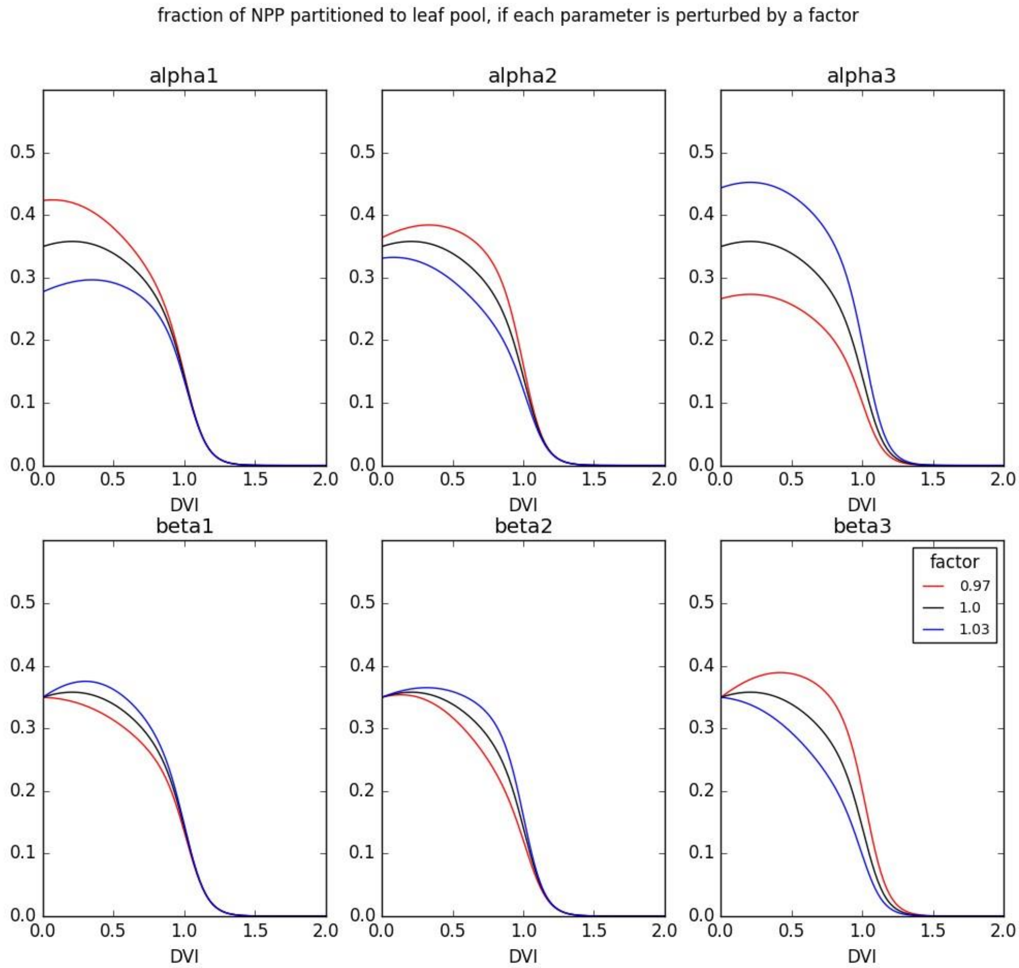

Fig S1: The fraction of NPP partitioned to leaf pool, when partitioning parameters are perturbed by a factor in the sensitivity analysis.