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Calibration and evaluation of JULES-crop for maize in Brazil

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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 = .73 and .71, respectively, for summer season and off-season datasets), crop height (EF = .89), and grain dry mass (EF = .61 and .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 = .39) and soil moisture (EF = .44), demonstrating the necessity of further improvements including additional parametrizations of the rainfed conditions.

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).

Abbreviations: DVI, development index; EF, efficiency index; JULES, Joint UK Land Environment Simulator; LAI, leaf area index; NPP, net primary productivity; PBCM, processed-based crop model.

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.

Core Ideas

- JULES-crop was calibrated for maize in different regions of Brazil, cultivars, and water management conditions.
- The model well simulated the crop phenology, crop height, leaf area index, and grain dry mass.
- Simulations for leaf dry mass and soil moisture in rainfed conditions still need improvement.

2 | MATERIALS AND METHODS

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:

$$T_{\text{eff}} = \begin{cases} 0 \text{ for } T < T_{\text{b}} \\ T - T_{\text{b}} \text{ for } T_{\text{b}} \le T \le T_{\text{o}} \\ (T_{\text{o}} - T_{\text{b}}) \left(1 - \frac{T - T_{\text{o}}}{T_{\text{m}} - T_{\text{o}}}\right) \text{ for } T_{\text{o}} < T < T_{\text{m}} \\ 0 \text{ for } T \ge T_{\text{m}} \end{cases} \quad (1)$$

where T_{o} is optimal temperature for crop development; T_{m} is maximum temperature for crop development, T_{b} 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 C pool (π), Equation 2 was used:

$$\pi = \frac{\exp(\alpha_i + \beta_i \mathrm{DVI})}{\sum_j \exp(\alpha_j + \beta_j \mathrm{DVI})} \quad (2)$$

where j = stem, leaf, harvest, and root. α_i and β_i 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 C 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 leaf area index (LAI). This occurs when DVI becomes greater than the parameter controlling the senescence phase ($\mathrm{DVI_{sen}} = 0.4$) (Equation 3):

$$\mathrm{sen_{dvi}} = \mu\left(\mathrm{DVI} - \mathrm{DVI_{sen}}\right)^{\nu} \quad (3)$$

where μ and ν allometric coefficients for calculation of senescence.

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

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

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

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

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

where $\mathrm{C_{leaf}}$ 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 C, 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 $\mathrm{C_{stem}}$ pool is used to calculate the crop height (h) (Equation 6):

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

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

2.2 | 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, 22°42′30″ S, 47°38′30″ W; 546 m asl). Of these four experiments, one was carried out for this study and the other three were carried out by T. 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°21′33″ S, 3°44′26″ W; 93 m asl); (b) the research and extension unit of State University of São Paulo, located in Selviria, State of Mato Grosso do Sul (Midwest region, 20°22′11″ S, 51°25′9″ W; 345 m asl); 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, 30°5′9″ S, 51°37′5″ W; 18 m asl).

The climate in Piracicaba is classified by Köppen (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 1.

In all experiments, detailed crop growth variables were monitored, including leaf dry mass, stem dry mass, grain dry mass, crop height, and LAI, as described by T. 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. In Exp. 4, soil moisture data was measured using a frequency domain reflectometry (FDR) probe (Diviner 2000), calibrated for the local soil for the 0-to-60-cm depth (Marin et al., 2020).

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 3. For other locations, it was used for the WATCH dataset based on ERA-Interim (WFDEI) re-analysis data contemplating meteorological data from 1979 to 2016 (Weedon et al., 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 1 Description of the experimental databases used for Joint UK Land Environment Simulator (JULES)-crop calibration in four different regions of Brazil

Experiment	Region	County	Sowing and harvest dates	Cultivar, varieties or hybrid	Treatments	Temperature and precipitation[a]	Water regime	Row spacing	Plant population	References
								m		
1	Southeast	Piracicaba	29 Nov. 2018 and 28 Mar. 2019	DKB363	Summer season	24.9 °C, 847.4 mm	Irrigated	0.45	66,000	—
2	Southeast	Piracicaba	7 May 2016 and 18 Oct. 2016	P4285YH	Off-season	19.2 °C, 653.6 mm	Irrigated	0.45	66,000	T. Souza et al. (2019)
3	Southeast	Piracicaba	10 June 2016 and 19 Oct. 2016	P4285YH	Off-season	19.3 °C, 374.6 mm	Rainfed	0.9	70,000	T. Souza et al. (2019)
4	Southeast	Piracicaba	5 Dec. 2019 and 30 Mar. 2020	LG36790	Summer season	24.9 °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 °C, 511 mm	Irrigated	0.75	67,000	França et al. (1999)
6	Northeast	Chapadinha	20 Feb. 2015 and 4 June 2015	AG 1051	Summer season	26.15 °C, 897 mm	Rainfed	0.85	58,823	K. Santos (2016)
7	Midwest	Selviria	2 Dec. 2014 and 6 Apr. 2015	DKB393	Summer season	27.4 °C, 1,058 mm	Rainfed	0.45	65,000	Rosa (2017)

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

TABLE 2 Soil physical parameters required by Joint UK Land Environment Simulator (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}	1.27×10^6	1.26×10^6	1.26×10^6	1.37×10^6
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

TABLE 3 Meteorological variables required by Joint UK Land Environment Simulator (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, ˚C
Wind	Wind speed, m s^{-1}
Pstar	Air pressure, Pa
Q	Specific humidity, kg kg^{-1}
diff_rad	Diffuse radiation, W m^{-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 (Tables 1–3). 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 C fixation capacity.

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 1), and the second for off-season maize cultivars, which corresponds to the P4285YH cultivar (Table 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 2.3, 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 other parameters considered to be well-known,

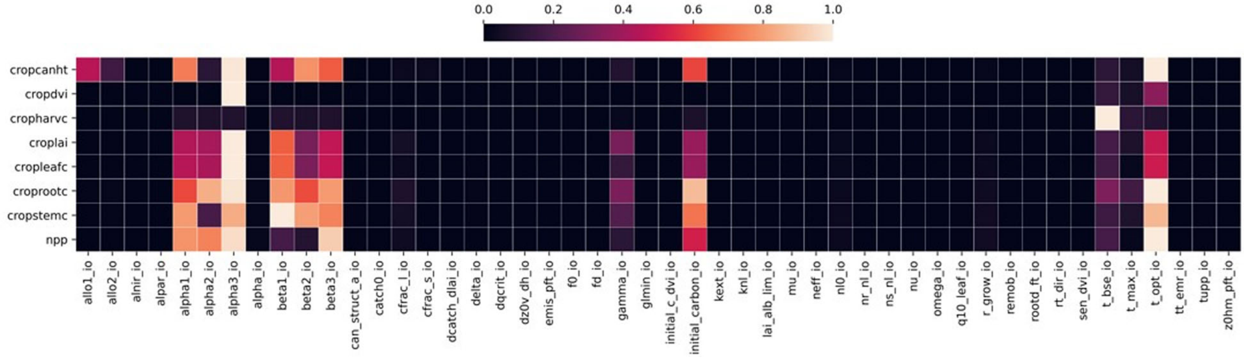

FIGURE 1 Heatmap of the local sensitivity analysis of the Joint UK Land Environment Simulator (JULES)-crop parameters for the Exp. 1 (Piracicaba, SP). Greater sensitivity is expressed by values closer to 1 and clearer colors

such as the base temperature (t_base_io), optimum temperature (t_opt_io), and others related in the supplemental material. 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 RMSE and mean absolute error (MAE) (Loague & 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 overall statistical indices for both groups of summer and off-season cultivars. All other model parameters were kept at the values from Williams et al. (2017).

3 | RESULTS AND DISCUSSION

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 Exp. 1 (Southeast; Table 1). Twenty-eight are associated with the model functionality to simulate C4 vegetation (Supplemental Table S1) and 24 are associated with the specific crop parametrization of JULES-crop (Supplemental Table S2), based on the output variables described in Section 2.3: LAI, crop height, crop development index, the C 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) (Figure 1). These parameters vary according to the DVI, a model variable used for calculating plant C 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 NPP variables (Figure 1; Supplemental Figure S1).

The fact that the leaf-related partition parameters are more sensitive than the others may be related to the difference in C allocation for this structure. According to Nabinger and Pontes (2002), the balance between photosynthesis and respiration generates a quantity of C 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 family is uneven to meet the internal demand of the plant, with the formation of leaves mainly in vegetative stage, when more C will be allocated due to the need for the plant to have a leaf area to intercept solar radiation, in comparison to the C 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 NPP. Because NPP affects the leaf C, and thus LAI (as described in Section 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 effect on estimating the output variables.

Two sensitive parameters in the analysis were the base and optimum temperatures (t_base_io and t_opt_io, Figure 1). The JULES-crop simulation is based on the DVI, that is, 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 C partitioning parameters. Another sensitive parameter observed was related to

TABLE 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)

Parameter	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

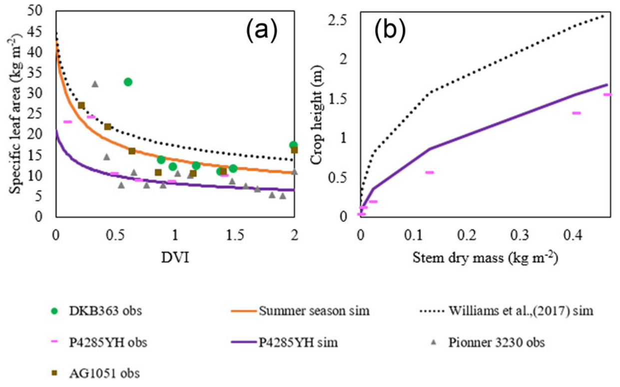

FIGURE 2 Calibrations for (a) specific leaf area and (b) crop height derived for different maize experiments conducted in four Brazilian regions. Off-season maize observations are those from cultivar P4285YH

initial amount of C in crops (Figure 1), as this experiment did not measure the C 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.

3.2 | JULES-crop calibration

Compared with the parameter values reported by Williams et al. (2017) when assessing maize cultivars in Nebraska, we found greater differences for cultivar P4285YH, which is commonly used for off-season crops after soybean [*Glycine max* (L.) Merr.] crop in tropical-producing regions of Brazil (Table 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 C allocation (Liang et al., 2020; Peng et al., 2018), 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 4).

The C partition parameters were derived using the observed data as a reference (Figures 2 and 3). In comparison to off-season cultivars, most parts of observed partitioning fractions for the summer season cultivars were shifted to higher DVI (Figure 2a) points, with the exception of the Pionner 3230 cultivar (South, Exp. 5) when DVI was between 0.5 and 1 and 1.5 and 2, so we also calibrated SLA for the two periods of crop production separately (Figure 2a, colored lines). Once again, this effectively mimicked the shifted pattern in DVI. The crop height measurements (Figure 2b) were taken only during the off-season experiment (T. Souza et al., 2019), so we adopted the same crop height parameters values (Table 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 C partitioning (Figure 3) and SLA (Figure 2a) indicate some water and thermal stress effect in grain dry mass yield (Figure 3d), specifically in the cultivars DKB363 (Midwest, Exp. 7), AG1051 (Northeast, Exp. 6), and LG36790 (Southeast, Exp. 4), inducing the C allocation for different structures as a strategy to supply the atmospheric water demand. In the DKB363 (Midwest, Exp. 7), AG1051 (Northeast, Exp. 6), and LG36790 (Southeast, Exp. 4), both under rainfed conditions, the flowering occurred when the air temperature exceeded the 33˚C, which was above the optimum temperature of 28˚C and influencing the C allocation in view of the negative effects on the crop (Johkan et al., 2011). We verify that in Exp. 6 and 7 (Northeast and Midwest) the root C partitioning is extended after the flowering stage (DVI > 1) resulting in less C in the grain (Figure 3a,d). Such ecophysiological strategy was also observed by Pedreira et al. (2001) and Duan et al. (2019) in Poaceae species, with a greater proportion of C allocated to the root system in relation to the aboveground parts as an effect of deepening the root system towards water and nutrients. Although crop models based on fixed C 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.

We also observed a greater fraction of C partitioned to leaves (Figure 3c) in the knee-high stage of the off-season cultivar (for DVI < 0.5) than in the summer season one, with a C partitioning around 50% allocated to leaves in the off-season cultivar in comparison to the summer cultivars, for which the C partitioning ranged from 30 to 45% for DKB363 (Southeast, Exp. 1) and Pionner 3230 (South, Exp. 5), respectively. Liang et al. (2020) observed, in two maize cultivars, a decrease of 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 C retained in leaves in our

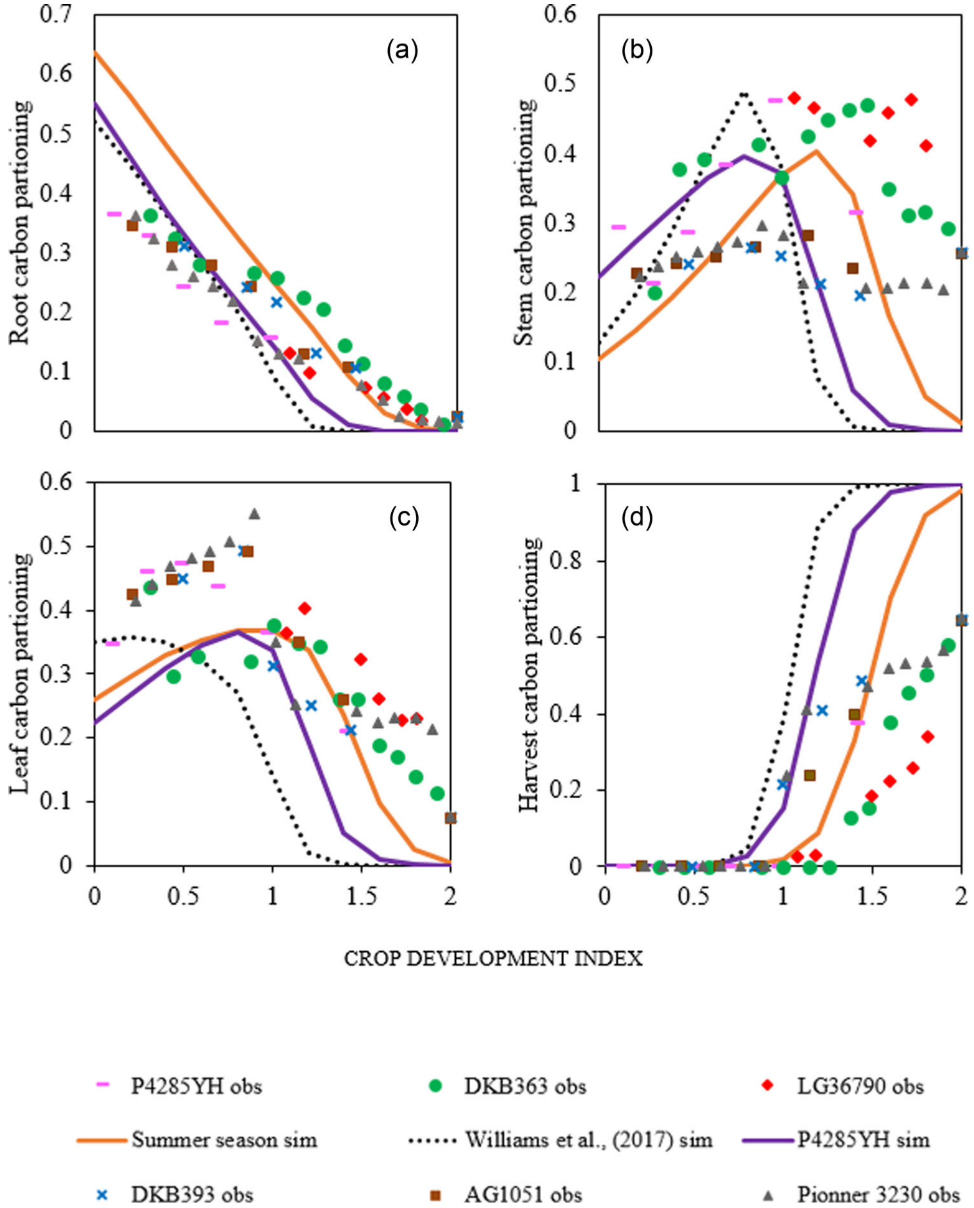

FIGURE 3 Carbon partitioning fractions for the (a) root, (b) stalk, (c) leaf, and (d) grain C pools, derived for different maize experiments conducted in four Brazilian regions. Off-season maize observations use cultivar P4285YH

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 differences in the stem height and mass (Figure 3b), these being greater in some summer cultivars than in the off-season, with C allocation to stems ranging from 20 to 40%, at the end of the season (DVI > 1.5) in cultivars specifically in DKB363 (Southeast, Exp. 1) and LG36790 (Midwest, Exp. 7). However, in the tasseling stage (DVI = 1) occurred the greater stem C allocation for off-season cultivar (Figure 3b), reaching 48% of the C distributed for the stem. Although our results contrast with off-season and Williams et al. (2017), similar C allocation rates at the end of the 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 Section 3.1 summarizes the importance of modifying the C allocation to calibrate JULES-crop for different cultivars and sowing dates.

3.3 | Evaluation of the JULES-crop calibration

JULES-crop simulated maize development and growth, as well as plant structures and C pools during the crop cycle

TABLE 5 Statistical indexes of performances of the calibrated Joint UK Land Environment Simulator (JULES)-crop model in simulating leaf, stalk, and grain dry mass, leaf area index (LAI), canopy height, and soil moisture in four Brazilian regions, Brazil

Variable	R^2	*d*-index	RMSE	EF
		Mg ha^{-1} m^2 m^{-2}, m, or cm^3 cm^{-3}		
Summer season				
Stem dry mass	.92	.86	1.12	.54
LAI	.96	.91	0.59	.73
Leaf dry mass	.89	.75	1.13	.39
Grain dry mass	.94	.93	1.31	.61
Soil moisture	.78	.81	0.01	.44
Off-season				
Leaf dry mass	.89	.71	0.46	.63
Stem dry mass	.93	.91	0.98	.71
LAI	.95	.98	0.34	.71
Grain dry mass	.96	.94	1.03	.89
Crop height	.96	.98	0.18	.88

Note. EF, efficiency.

(Table 5; Figures 4 and 5) satisfactorily, in two different conditions (irrigated and rainfed) in different regions of Brazil. Using the same dataset collected for an off-season cultivar, T. Souza et al. (2019) calibrated the DSSAT-CERES Maize and found EF = .70 for LAI in irrigated conditions, which is similar to this study (EF = .71 in off-season cultivar and EF = .73 in summer cultivar). JULES-crop showed higher efficiency for simulating crop height in both treatments: EF = .70 and .68 for irrigated and rainfed conditions found by T. Souza et al. (2019) in comparison to .88 found in this study (Table 5). Thus, LAI and canopy height were better simulated compared with other variables (Table 5; Figures 4, and 5b,c); moreover, it is important to highlight the grain dry mass simulation in summer cultivars (EF = .61 for summer experiment and EF = .89 for off-season experiment) observed in Table 5 and Figure 4d. Important to mention despite the difference between the harvest C partitioning for both seasons and observed data (Figure 3d) the model simulated grain yield with accuracy and efficiency, such as high observation plots along the bottom line (Table 5; Figures 3d, 4d, and 5d). The difference can be explained because JULES-crop remobilizes C 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 Figure 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.

Soil moisture presented the second lowest value of efficiency in this study (EF = .44 and R^2 = .78, Table 5). However, this is a higher value compared with the model CropSPAC, as observed by Duan et al. (2019) that demonstrate a R^2 = .78 and EF = .26. JULES-crop also obtained a better statistical index than M. Santos et al. (2020), 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 with the RMSE of 0.01 cm^3 cm^{-3} found in this study. Furthermore, they found an average *d*-index of .58 while this study obtained *d*-index = .81. Inaccuracies for soil moisture simulations are common in crop models that use 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, Exp. 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 5; Figures 4f and 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, Exp. 4), AG1051 (Northeast, Exp. 6), and DKB393 (Midwest, Exp. 7) were conducted under rainfed conditions, and DKB363 (Southeast, Exp. 1) and Pionner 3230 (South, Exp. 5) under irrigation. The rainfed cultivars showed different C allocation for leaves compared with 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 5) might be the canopy structure differences among cultivars due to the genetic diversity, in addition to the high sensitivity demonstrated in the leaf C 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 = .63 for off-season and EF = .39 for summer calibration).

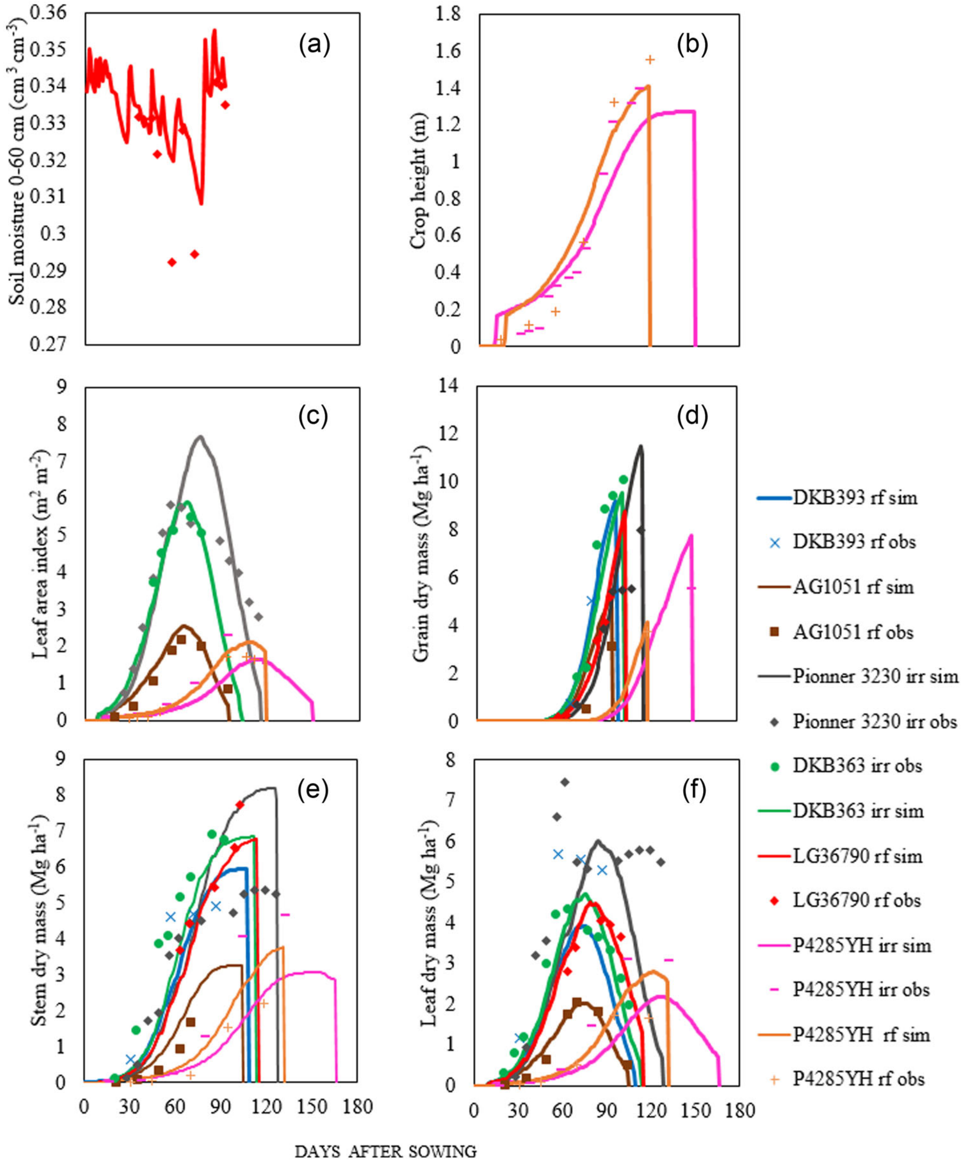

FIGURE 4 Comparison between observed and simulated variables by Joint UK Land Environment Simulator (JULES)-crop for (a) soil moisture, (b) crop height, (c) leaf area index (LAI), (d) grain dry mass, (e) stem dry mass, (f) leaf dry mass of different maize cultivars in different regions of Brazil. Irr-Irrigated, rf-rainfed, obs-observed, sim-simulated. Off-season maize observations use cultivar P4285YH

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 C 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 the 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 5; Figures 4 and 5c), crop height (Table 5; Figures 4 and 5c), and grain dry mass (Table 5; Figures 4 and 5d). High efficiency in grain dry mass is important for the use 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.

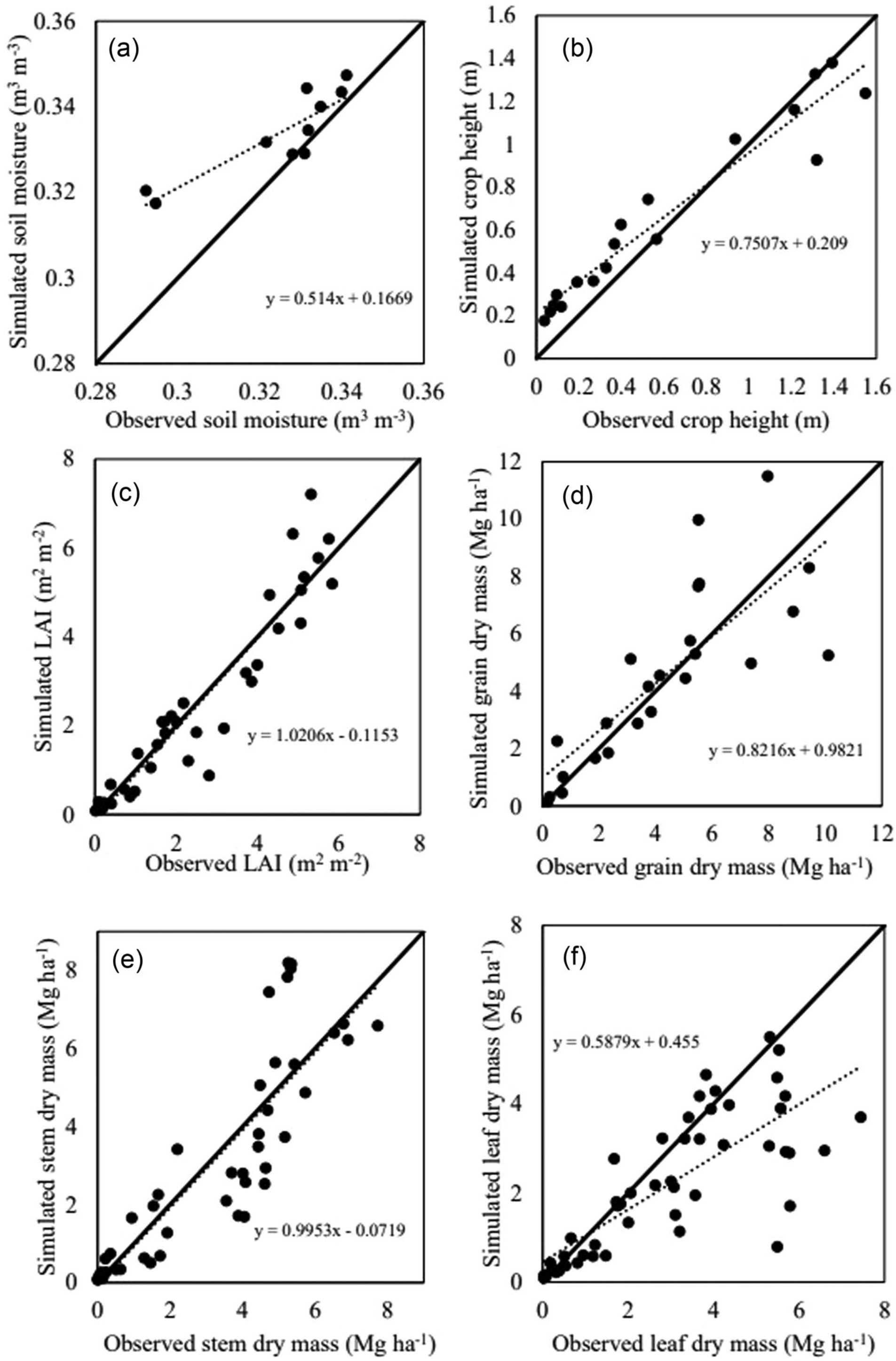

FIGURE 5 Relationship between simulated and observed values for (a) soil moisture, (b) crop height, (c) leaf area index (LAI), (d) grain dry mass, (e) stem dry mass, (f) leaf dry mass of maize for different regions of Brazil

4 | CONCLUSION

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 C partitioning and the parameters associated to the crop specific leaf area. The JULES-crop well simulated the C partitioning and allometric relationships for different maize cultivars in Brazil under irrigated and rainfed regimes, for summer and off-season sowing dates. The JULES-crop performance for simulating the development of maize crop in the field experiments was satisfactory, particularly for crop height

(EF = .89), LAI (EF = .73 and .71, respectively, for summer and off-season experiments) grain dry mass (EF = .61 and EF = .89, respectively, for summer and off-season experiments). However, it demonstrated a low efficiency simulating the leaf dry mass (EF = .39) and soil moisture (EF = .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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AUTHOR CONTRIBUTIONS

Amauri Cassio Prudente Junior: Conceptualization; Investigation; Data curation; Formal analysis; Validation; Writing original draft; Writing –review & editing. Murilo S. Vianna: Methodology; Software; Writing original draft; Writing – review & editing. Karina Williams: Software; Writing original draft; Writing – review & editing. Marcelo V. Galdos: Resources; Writing original draft; Writing – review & editing. Fabio R. Marin: Conceptualization; Methodology; Formal analysis; Supervision; Visualization; Resources; Writing original draft; Writing – review & editing.

CONFLICT OF INTEREST

The authors declare no conflicts of interest.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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