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Implications of water management on methane emissions and grain yield in paddy rice: A case study under subtropical conditions in Brazil using the CSM-CERES-Rice model

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ABSTRACT

Rice (*Oryza sativa* L.) is a staple food and plays a crucial role in the food security of many countries. However, rice cultivation is associated with significant methane (CH_4) emissions, contributing to overall greenhouse gas emissions and, thus, climate change. In this context, process-based crop models are useful tools for understanding and predicting the complex interactions between crop production, environmental factors, and sustainability. The objective of this study was to evaluate the performance of the Cropping System Model (CSM)-CERES-Rice model and DSSAT-GHG module to predict daily methane emissions and rice grain yield for different irrigation practices in a subtropical environment. The study employed a comprehensive approach, including measurements of daily CH_4 emissions, phenological stages, final aboveground biomass, and grain yield for rice cultivars BRS Pampa, BRS Pampeira, A705, and XP113 conducted over four consecutive crop seasons (2019–2023) and two irrigation systems: continuous flooding (CF) or alternate wetting and drying (AWD) in Capão do Leão, RS, Brazil. We followed a four-step methodology involving initial calibration of cultivar parameters, sensitivity analysis (soil-related parameters associated with CH_4 emissions), final cultivar parameters calibration, and long-term simulation analysis. Based on the sensitivity analysis and comparison to observed emissions, modifications were made to soil-related parameters such as soil buffer regeneration after drainage events (BRAD) and the fraction of soil water-filled porosity above which methane production occurs ($WFPS_{thresh}$) to enhance the accuracy of methane production. Optimal parameter combinations ($WFPS_{thresh}$ = 70 %, BRAD = 0.070 d^{-1}) were selected based on a comparative analysis, enabling CH_4 simulations under non-flooded conditions. The predictive capability of the CERES-Rice model exhibited an average bias for grain yield of 485 kg ha^{-1} under CF and 592 kg ha^{-1} under AWD conditions. The results showed that the GHG module of DSSAT, after BRAD and $WFPS_{thresh}$ parameter adjustments, was able to simulate daily CH_4 emissions in paddy rice with a very good agreement (average index of agreement (D-Statistic) of 0.87 for CF and 0.70 for AWD). Following the model evaluation, long-term simulations for different irrigation practices revealed the impact on grain yield, cumulative methane emissions, and seasonal applied irrigation. The highest crop water-methane productivity (CWMP = 52 %) was observed under sprinkler irrigation at 50 % soil water depletion, identifying it as the most sustainable option in this subtropical environment. Thus, the CSM-CERES-Rice model combined with the DSSAT-GHG module proved to be a potential tool for agricultural and environmental management of rice fields under subtropical conditions.

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1. Introduction

Rice (*Oryza sativa* L.) is a major food staple in the diets of a significant portion of the population across Asia, Latin America, and, increasingly, in Africa. Global rice production reached 513,744 Mg in 2022 and is projected to rise to 570,000 Mg within the upcoming decade (USDA, 2023; OECD-FAO, 2023). About 57 % of global rice production is concentrated in subtropical or temperate regions, mainly from the lowlands (Gadal et al., 2019). Brazil achieved a total rice production of 11,660 Mg in 2022, establishing itself as the leading non-Asian rice producer, with more than 80 % of production concentrated in the south of the country under subtropical conditions, with most rice production from lowlands (USDA, 2023; CONAB, 2023).

Rice cultivation in the lowlands of Brazil presents a complex array of challenges, notably navigating the intricate synergy among grain yield, soil and water management, and environmental impact. The conventional system of flooded rice cultivation typically encompasses intensive soil tillage practices, such as plowing, harrowing, land leveling, and constructing levees for irrigation (Theisen et al., 2018; Sousa et al., 2021). Generally, these soils exhibit shallowness, poor natural drainage characterized by almost impermeable subsurface horizons, a high soil bulk density, a low total porosity with a high micro/macropores ratio, and the presence of compacted layers (Streck et al., 2008; Almeida, 2023). Furthermore, these conditions, mainly for continuous flooding (CF) systems, engender an environment that is conducive to the genesis and subsequent emission of methane (CH_4) — a greenhouse gas with a significantly higher potential for global warming compared to carbon dioxide (Conrad, 2020; Gupta et al., 2021; Harrison et al., 2021; Silva et al., 2021). Despite the acknowledgment of methane emissions from rice paddies, there is a lack of detailed examination of existing studies that have explored the complexities of methane emissions under different management practices under subtropical conditions.

Water-saturated soils or continuous flooding are the primary cause for methane emissions; under these conditions, methanogenic microbial processes can be alleviated through the oxygenation of soils (Angle et al., 2021; Yuan et al., 2023). A method to increase the oxygenation of rice paddies is an irrigation management practice referred to as alternate wetting and drying (AWD), which has been extensively studied in several rice-producing regions of the world (*e.g.* Song et al., 2021; Volpe et al., 2023). In AWD, rice paddies are managed with intermittent flooding (alternate cycles of saturated and unsaturated soil conditions), where irrigation is interrupted. The soil is either allowed to drain or water content is allowed to subside until it reaches a specific moisture level, after which the soil is reflooded (Carrijo et al., 2017; Sousa et al., 2021). Some studies reported that AWD reduced global warming methane release by 15–90 % compared to continuously flooded systems depending on soil texture, amendments, or the ecosystem carbon balance (Linquist et al., 2015; Haque et al., 2021; Ariani et al., 2022). Additional mitigation strategies include the use of plastic film mulching (Liu et al., 2021), biochar amendments (Nan et al., 2020), optimizing drainage time (Souza et al., 2021), rice breeding techniques (Rajendran et al., 2023).

Field data can be synergistically utilized in conjunction with process modelling simulations within specific environments to enhance our understanding of the processes governing paddy rice water management and methane emissions. Existing models, such as the DNDC (Gilhespy et al., 2014), APSIM (Holzworth et al., 2014), DayCent (Parton et al., 1994), and STICS (Beaudoin et al., 2023) have been employed to predict CH_4 emissions from rice paddies (Guo et al., 2023; Tang et al., 2024). The Cropping System Model (CSM)-CERES-Rice (Singh et al., 1993; Ritchie et al., 1998) is part of the Decision Support System for Agrotechnology Transfer (DSSAT) (Jones et al., 2003; Hoogenboom et al., 2019). The CERES-Rice model simulates rice growth across a wide range of environmental and management conditions (*e.g.,* Ahmad et al., 2013; Gao et al., 2020; Darikandeh et al., 2023). Recently, the greenhouse gas (GHG) module was integrated into DSSAT version 4.8, which added GHG emissions simulation in the soil carbon balance, including methane, nitrous oxide (N_2O), and carbon dioxide (CO_2).

The simulation of GHG emissions represents a significant enhancement towards improving crop models as indispensable tools for agricultural management, thereby adding a crucial dimension to sustainability practices. Nevertheless, as this tool is relatively new, it requires testing and refinement to ensure accurate simulations. This study addresses this scientific gap by utilizing DSSAT-GHG module, which provides a novel opportunity to simulate methane emissions in rice systems. By incorporating field-measured data and conducting sensitivity analyses on key parameters, we aim to refine the model's capacity to simulate methane emissions under different water management practices. Additionally, our study seeks to evaluate alternative management strategies to mitigate methane emissions in subtropical lowland rice systems in Brazil, a topic currently underrepresented in both the literature and existing simulations.

We hypothesize that a comprehensive examination of the DSSAT-GHG module's source code, coupled with sensitivity analysis and comparison to field-measured data, can contribute to model enhancement. The objectives of this study encompass (i) analyzing the DSSAT-GHG module, (ii) conducting sensitivity analysis on the identified key parameters, (iii) calibrating and assessing the performance of the CSM-CERES-Rice model in simulating rice growth, development, and particularly CH_4 emissions; and (iv) applying long-term simulations using different water management.

2. Materials and methods

2.1. Field experiments

Irrigated rice experiments were conducted in Capão do Leão (31°52′S, 52°21′W, 13 m.a.s.l), Rio Grande do Sul, southern Brazil, during four cropping seasons between 2019 and 2023: (i) S1 - 2019/2020, (ii) S2 - 2020/2021, (iii) S3 - 2021/2022, (iv) S4 – 2022/2023. The climate classification for Capão do Leão is Cfa (humid subtropical, no dry season climate). Daily weather data for Capão do Leão were obtained from the Embrapa Temperate Agriculture on-site automatic weather station. For the automatic weather stations, the following daily variables were measured: (i) total solar radiation (MJ m^{-2} day^{-1}); (ii) maximum and minimum air temperatures (ºC); and (iii) rainfall (mm).

Fields were cultivated with rice cultivars, BRS Pampa, BRS Pampeira, A705, or XP113 at a plant density of 300 plants m^{-2} under conventional tillage practices and fertilization management was performed according to pre-established applications based on soil analysis (Table 1). The experiments included two distinct irrigation treatments: 1) continuous flooding, where fields were consistently submerged in water, and 2) alternate wetting and drying irrigation, involving cyclic wetting, and drying of each field. More information about crop management for these locations can be found in Scivittaro et al. (2023).

Throughout all cropping seasons, the experimental plots were established with two irrigation practices (CF and AWD) combined with four rice cultivars (BRS Pampa, BRS Pampeira, A705, and XP113). The plots were arranged in a randomized complete block design with five replications. Although the cultivars differed across the four cropping seasons, each was repeated for at least two cropping seasons (Table 1). Daily CH_4 emissions, phenological stages (following the methodology described by Counce et al. (2000), final grain yield, and aboveground biomass at harvest were collected for all experiments. The grain yield and final aboveground biomass measurements collection area were standardized at 9.5 m^2 for each replication. The phenological stages were measured only under CF conditions.

For a collection of CH_4 emissions, the static closed chamber method described by Mosier (1989) was used. This method involves a temporarily sealed system in which gas is sampled at 0, 5, 10, and 20 minutes after chamber closure. Consequently, this is interpreted as continuous gas concentration changes, as Denmead and Raupach (1993)

Table 1
Description of field experiments conducted in Capão do Leão during four cropping seasons from 2019 to 2023.

Cropping season	Cultivar	Sowing date	Harvest date	Fertilization at sowing (kg ha^{-1}) [a]	1st Top-up fertilization (kg ha^{-1})	2nd Top-up fertilization (kg ha^{-1})
S1–2019/2020	BRS Pampa	Nov 12	Mar 23	300	90 urea	45 urea
	XP113	Nov 12	Mar 20	(5−20−20)	40 K_2O	
S2–2020/2021	BRS Pampa	Dec 11	Mar 15	450	90 urea	45 urea
	A705	Dec 11	Mar 15	(5−20−20)	40 K_2O	
	BRS Pampeira	Dec 11	Apr 04			
S3–2021/2022	BRS Pampa	Oct 23	Mar 03	420	80 urea	45 urea
	A705	Oct 23	Mar 03	(2−18−18)		
	XP113	Oct 23	Mar 07			
	BRS Pampeira	Oct 23	Mar 11			
S4–2022/2023	BRS Pampa	Nov 17	Mar 21	340 (5−20−20)	85 urea	48 urea

[a] The notation 5–20–20 or 2–18–18 represents the percentage of nutrient content in the fertilizer mixture. It provides information about the proportions of nitrogen (N), phosphorus (P), and potassium (K) contained within the fertilizer. The reported rates are associated with the applied fertilizer and do not reflect the nutrient equivalent.

highlighted. The collection systems consist of aluminum chambers positioned on bases, creating a hermetic enclosure through the presence of water in the upper channel of the bases, where the chambers rest, as detailed by Gomes et al. (2009). As the rice plants grew, one or two extensions were utilized, as required, positioned between the top and the base of the collection system.

The air samples were collected during the time from emergence until final harvest, from each replication at approximately 7-day intervals for CF and 3-day intervals for the AWD treatment. Air samples within the chambers were homogenized for 30 seconds using fans located and manually extracted using 20 mL polypropylene syringes with Luer Lock valves. These samples were collected at time intervals of 0, 5, 10, and 20 minutes after chamber closure, consistently between 9 and 11 AM, to represent daily greenhouse gas emissions most accurately (Costa et al., 2008). Subsequently, the air samples were conveyed to the Environmental Biogeochemistry Laboratory of the Federal University of Rio Grande do Sul. Methane concentrations were determined using gas chromatography on a Shimadzu GC-2014 chromatograph. The chromatograph had a packed column operating at 70°C and a flame ionization detector (FID) operating at 250°C. Methane quantification was achieved using N_2 as the carrier gas, flowing at a rate of 26 mL min^{-1}.

2.2. Crop model simulations

The CSM-CERES-Rice model in DSSAT v.4.8 (Hoogenboom et al., 2019, 2024) was used in this study. Using a modular structure, this model simulates the growth, development, grain yield, and dynamics of soil water, carbon, nitrogen, phosphorus, and greenhouse gas emissions over the rice crop season (see Jones et al., 2001). Furthermore, the model can simulate the water and nitrogen balance in rice fields conducted under flooded systems, upland conditions, or alternate wetting and drying conditions (Timsina and Humphreys, 2006).

The soil water balance and soil organic matter are crucial for understanding the CH_4 emissions process. DSSAT computes carbon balance using the CERES-based organic carbon model (Godwin and Jones, 1991) or the DSSAT-CENTURY model (Parton et al., 1994; Gijsman et al., 2002; Porter et al., 2010) with DSSAT-CENTURY as the default option for rice; these two distinct approaches comprehensively assess carbon dynamics within the agricultural system considering temperature and water factors, soil texture, and cultivation practices. In this study, we run all simulations using DSSAT-CENTURY. The DSSAT-CENTURY method introduces a more detailed categorization of organic residues as surface litter or soil litter. These categories further differentiate into easily decomposable metabolic materials and recalcitrant structural materials based on the lignin/N ratio. The structural portion of the crop residue/litter has a fixed C/N ratio of 200, while the C/N ratio of metabolic material varies with litter N concentration (Gijsman et al., 2002). The decomposition of metabolic material contributes to the active SOM pool (SOM1) in both surface and soil layers; structural material (fibrous and easily decomposable components) with the latter becoming part of the surface or soil SOM1 and the former joining the intermediate SOM pool (SOM2). SOM1 decomposes into SOM2, while soil SOM1 decomposes into passive SOM (SOM3); SOM2 can further decompose into SOM3 or reactivate as soil SOM1 (Gijsman et al., 2002). The SOM3 is estimated based on stable organic C, field history and duration, or regression equation (see Porter et al., 2010; Godwin and Singh, 1998 for more details).

Our investigation into CH_4 emissions simulations with the DSSAT-GHG module in paddy rice began with the BRS Pampa cultivar. We calibrated BRS Pampa and assessed the crop model's performance in simulating grain yield, crop phenology, aboveground biomass, and CH_4 emissions. Upon evaluating the simulated data against field data, we observed that the model consistently simulated methane emissions as zero under AWD conditions during the four cropping seasons, contrary to the field observations. Thus, we initiated a protocol to investigate the causes of DSSAT-GHG consistently simulating that there are no methane emission values under AWD conditions and to propose means for improving methane simulation accuracy.

We defined a four-step protocol (Fig. 1): (i) step 1, we calibrated cultivar parameters for the BRS Pampa cultivar; (ii) step 2, we reviewed the DSSAT-GHG module and conducted a sensitivity analysis for parameters related to soil, specifically those associated with soil buffer regeneration after drainage events (BRAD) and the fraction of soil water-filled porosity above which methane production occurs ($WFPS_{thresh}$); (iii) step 3, we further calibrated the cultivar coefficients for BRS Pampa, BRS Pampeira, A705, or XP113, using the best-performing combination of BRAD and $WFPS_{thresh}$ obtained in step 2. The cultivar calibrations were evaluated based on phenology, grain yield, aboveground biomass in the field, and CH_4 emissions under both CF and AWD irrigation conditions; (iv) step 4, we utilized the model to simulate long-term methane emissions and water use scenarios under different irrigation practices.

2.3. Step 1: BRS Pampa calibration

Calibration of the cultivar coefficients for the BRS Pampa cultivar was conducted using the experimental data from Capão do Leão for the 2020/2021 season (S2) under continuous flooding. The calibration procedures for all the following steps were conducted by a trial-and-error method against observed values (phenological stages, grain yield, and final aboveground biomass). First phase, simulations were evaluated using the default cultivar parameters defined in the genotype file using observed weather (Supplementary Materials – Figs. S1–S4), soil, fertilizer management (Table 1), and conventional tillage practices for each crop season. The soil water holding characteristics, such as permanent wilting point, field capacity, and field saturation for each soil

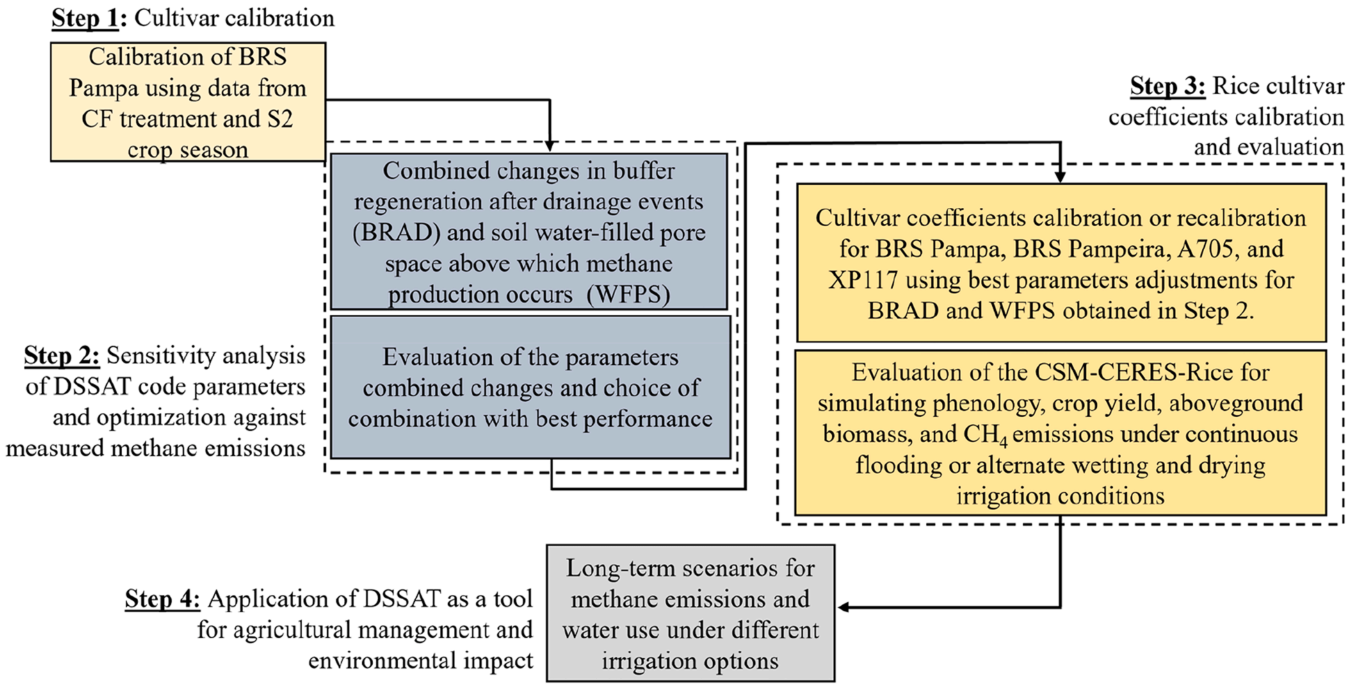

Fig. 1. Flowchart illustrating the methodology employed for simulating paddy rice systems in Capão do Leão using the CSM-CERES-Rice model. The flowchart is comprised of four primary steps: 1- BRS Pampa cultivar calibration using an experiment from crop season 2020/2021 (S2) conducted under continuous flooding (CF); 2- sensitivity analysis of DSSAT code parameters for methane emissions; 3- cultivar coefficients recalibration and evaluation for BRS Pampa, BRS Pampeira, A705, and XP113; and 4- application of DSSAT as a tool for agricultural management and environmental impact.

layer, were computed using pedotransfer functions obtained by Tomasella et al. (2000) for Brazilian soils. In the second phase, only the crop phenology coefficients (P1, P2O, P2R, and P5 – see description in Table 2) were calibrated based on observed phenological stages, specifically anthesis (R4) and physiological maturity (defined as R9). According to Counce et al. (2000), determining rice physiological maturity accurately with any morphological marker is challenging, if not impossible. Therefore, we chose to use R9 because it signifies the point at which all grains on the main stem panicle have elongated to the end of the hull. This event appears to represent physiological maturity in the model, as the physiological maturity date aligns with the end of grain dry matter accumulation. In the third and final phase, we calibrated the parameters G1, G2, and G3.

2.4. Step 2: sensitivity analysis of DSSAT code parameters and optimization against measured methane emissions

The sensitivity analysis was conducted with a specific focus on the methane emissions component within the CERES-Rice model. We reviewed the DSSAT-GHG module thoroughly, particularly concerning the interaction between soil water conditions and methane production calculations. The methane subroutine in DSSAT is based on the Arah model (Arah and Kirk, 2000), and we observed that methane simulations occur only during flooded conditions, while no emissions are simulated when a portion of soil pores is not saturated with water. This established assumption leads to simulated methane emissions consistently registering as zero during non-flooded times of AWD conditions. These simulated outcomes are not consistent from a realistic point of view. Yang and Chang (1998) found that methane production started when the soil water content reached 61 % of soil water holding capacity under

Table 2
Final values of the calibrated cultivar coefficients for BRS Pampa, BRS Pampeira, A705, and XP113 with data from Capão do Leão.

Traits	Definition	Unit	BRS Pampa	BRS Pampeira	A705	XP 113
P1	Time period from seedling emergence during which the rice plant is not responsive to changes in photoperiod.	Degree days (GDD)	390.0	271.0	255.0	174
P2O	Critical photoperiod or the longest day length at which the development occurs at a maximum rate.	Hours	11.5	12.6	12.2	11.5
P2R	The extent to which phasic development leading to panicle initiation is delayed for each hour increases in photoperiod above P2O.	GDD	32.0	110.0	80.0	234.0
P5	The period in GDD is from the beginning of grain filling to physiological maturity with a base temperature of 9°C.	°C d^{-1}	498.0	439.0	441.0	600.0
G1	Potential spikelet number coefficient as estimated from the number of spikelets per main culm dry matter.	Number g^{-1}	74.0	69.0	70.3	85.0
G2	Single grain dry matter (g) under ideal growing conditions.	g	0.027	0.025	0.023	0.040
G3	Tillering coefficient relative to IR64 cultivar under ideal conditions.	Scalar value	1.140	0.700	0.700	1.050
PHINT	Phyllochron interval, for each leaf-tip to appear under non-stressed conditions.	°C d^{-1}	60.0	55.0	55.2	55.0
THOT	Temperature above which spikelet sterility is affected by high temperature.	°C	32.0	32.0	32.0	32.0
TCLDP	Temperature above which spikelet sterility is affected by high temperature.	°C	16.0	16.0	16.0	16.0
TCLDF	Temperature below which panicle initiation is further delayed by low temperature.	°C	15.0	15.0	15.0	15.0

laboratory conditions. Other authors have verified methane emissions in paddy rice with partially saturated soil (*e.g.,* Sriphirom et al., 2019; Moterle et al., 2020; Zhang et al., 2020).

We investigated the methane subroutine and selected two parameters related to methane production under non-flooded conditions. The first parameter is a rate constant related to soil buffer regeneration after drainage events, it represents a fraction of water drainage per day. BRAD is employed in the calculation of reoxidation of the alternative electron acceptors (AEA_{red}) pool in the case of midseason drainage. In this scenario, the oxidation rate is correlated with the air-filled porosity (AFP) and maximum air-filled porosity (AFP_{MAX}). The original value for BRAD is set at 0.060 d^{-1}, obtained through trial and error (Matthews et al., 2000). This value means that the complete reoxidation of the AEA pool takes approximately 2 weeks (1 / 0.060 = 16.7 days). The second parameter was associated with AFP. The model outlined a condition in which AFP > 0 led to no CH_4 production, *i.e.*, CH_4 production occurs only under the condition of 100 % $WFPS_{thresh}$.

$$\frac{d[AEA_{red}]}{dt} = BRAD \times \frac{AFP_t}{AFP_{MAX} \times AEA_{red}} \quad (1)$$

The simulations for sensibility analysis were conducted for the BRS Pampa cultivar by varying BRAD combined with $WFPS_{thresh}$ parameters. The variation in BRAD, representing the inverse of the number of days required for recovery of soil buffer regeneration after drainage events, ranged dynamically. Lower values of BRAD corresponded to a more extended regeneration period, while higher values indicated a shorter regeneration period. The change from one BRAD value to the next represented a daily interval, with BRAD values spanning from 0.01 to 1.00 (or 1/BRAD from 1 to 100 days). Simultaneously, $WFPS_{thresh}$ parameters were adjusted in the range of 0–100 % in increments of 5 %. The sensitivity analysis was exclusively conducted under AWD conditions; it should be noted that sensitivity analysis under CF conditions would not provide meaningful insights, as all pores remain constantly filled with water ($WFPS_{thresh}$ = 100 %) throughout the inundation period. This resulted in 2000 combinations for each cropping season, *i.e.*, S1 to S4, generating 8000 sets of simulated daily CH_4 emissions compared to measured daily CH_4 emissions.

In this sensitivity analysis, we assess the DSSAT-GHG module's methane emissions response to changes in BRAD and $WFPS_{thresh}$. Subsequently, the simulated data were compared with the field-measured data, and we selected the BRAD and $WFPS_{thresh}$ values that resulted in greater model accuracy.

2.5. Step 3: rice cultivar coefficients calibration and evaluation

Calibration of the cultivar coefficients for the cultivars BRS Pampeira, A705, and XP113 and recalibration of BRS Pampa were conducted using the experimental data from Capão do Leão for the 2021/2022 (S3) growing season under continuous flooding conditions. The calibration was conducted by a trial-and-error method against observed values following the procedures described in the 2.1 section. All simulations were conducted using the Penman-Monteith potential evapotranspiration method (Allen *et al.*, 1998), the Suleiman–Ritchie soil water evaporation method (Suleiman and Ritchie, 2003), and the DSSAT-Century soil organic matter method (Parton et al., 1994; Gijsman et al., 2002). The cultivar traits obtained after the final calibration are shown in Table 2.

Initial soil moisture at the initiation of the simulation was set to field capacity, and soil analysis for each season defined ammonium (NH_4) and nitrate (NO_3) initial condition concentration. We also implemented the DSSAT-GHG module's source code changes on these simulations, using BRAD = 0.070 d^{-1} and $WFPS_{thresh}$ = 70 %, which showed the best performance. To evaluate the accuracy of the CERES-Rice model in predicting phenological stages, aboveground biomass, grain yield, and daily CH_4 emissions, the simulations were compared to measured data from field experiments.

2.6. Step 4: application of DSSAT as a tool for agricultural management and environmental impact

Following calibration and evaluation of the CSM-CERES-Rice model using experimental data, we applied the model to explore different irrigation practice scenarios in a long-term simulation analysis in Capão do Leão (Thornton and Hoogenboom, 1994). Our objective in these long-term simulations was to investigate which irrigation practice scenario is more sustainable for paddy rice under a subtropical environment, focusing on evaluating aspects of grain yield, water usage, and methane emissions. These scenarios encompassed the following irrigation treatments: (i) CF, continuous flooding; (ii) AWD, alternate wetting and drying; (iii) S-50 %, sprinkler irrigation initiated at 50 % of available soil moisture; (iv) S-60 %, sprinkler irrigation initiated at 60 % of available soil moisture, (v) S-80 %, sprinkler irrigation initiated at 80 % of available soil moisture, and (vi) S-90 %, sprinkler irrigation initiated at 90 % of available soil moisture. All sprinkler treatments were set up with 20 mm irrigation application rates.

The irrigation practices were assessed through the relationship between crop rice yield and factors of seasonal irrigation applied and cumulative methane emissions. We called this relationship here as crop water-methane productivity index (CWMP). CWMP was computed as the mean of three key ratios: (i) the ratio of maximum grain yield obtained in all long-term simulations to yield obtained for each season, (ii) the ratio of minimum seasonal applied irrigation obtained in all long-term simulations to seasonal applied irrigation simulated for each season, and (iii) the ratio of minimum cumulative CH_4 emission obtained in all long-term simulations to cumulative CH_4 emission simulated for each season (Eq. 2). This index served as a comprehensive indicator, shedding light on the intricate interplay between rice productivity, water resource utilization, and methane emission mitigation within various irrigation treatments. The index ranges from 0 % to 100 %, with values closer to 100 % indicating more efficient rice production in terms of water consumption and emitted methane.

$$CWMP = \text{mean}\left(\frac{\text{grain yield}}{\text{grain yield}_{MAX}} + \frac{\text{seasonal applied irrigation}_{MIN}}{\text{seasonal applied irrigation}} + \frac{\text{cumulativeCH}_4\text{emission}_{MIN}}{\text{cu mulativeCH}_4\text{emission}}\right) \times 100 \quad (2)$$

To configure these long-term simulations, we employed the settings from the experiment conducted with the BRS Pampa cultivar during the 2021/2022 season in Capão do Leão. The simulations were replicated over 30 crop seasons, using historical weather data spanning from 1990 to 2020. The assessment of long-term simulations focused on their influence on cumulative methane emissions, grain yield, seasonal applied irrigation, and CWMP.

2.7. Statistical analysis for model evaluation

The model's performance was assessed by comparing simulated with measured methane emissions, crop phenology, and grain yield from Capão do Leão. To gauge the goodness-of-fit, we employed several metrics: the root mean square error (RMSE) (Loague and Green, 1991), the index of agreement (D-statistic) (Willmott et al., 1985), and/or bias (B). RMSE was used to quantify the extent of error between the simulation results and the measured data. The D-statistic indicated how closely the model's predictions matched the actual observations; its values range from 0 to 1, with 0 indicating no agreement and 1 indicating perfect agreement between the model and observations. B measured the disparity between the final values predicted by the model and the actual observed values. When the model under-predicts, B is a negative value, while an over-prediction results in a positive B value. A high D-statistic, a low RMSE, and a B value approaching zero would indicate superior model performance. These statistics were calculated using the following formulas:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(s_i - o_i)^2}{n}} \quad (3)$$

$$D = 1 - \left[\frac{\sum_{i=1}^{n}(s_i - o_i)^2}{\sum_{i=1}^{n}(|s_i - \bar{o}| + |o_i - \bar{o}|)^2}\right], 0 \le D \le 1 \quad (4)$$

$$B = s_i - o_i \quad (5)$$

where n is the number of observations; s_i is the simulated value corresponding to measurement i on each date; o_i is observed value for measurement i; and $\bar{o}$ is the average of observed values.

3. Results and discussion

3.1. Sensitivity analysis of DSSAT parameters and optimization against observed methane emissions

The sensitivity analysis was conducted for two default parameters of the DSSAT-GHG module for the BRS Pampa cultivar over four crop seasons. The results showed that variations in the BRAD and $WFPS_{thresh}$ parameters could have a substantial impact on methane emission simulations for the AWD irrigation practice (Fig. 2). The variation of BRAD (d^{-1}) values resulted in a variation of the daily simulations; the outputs were plotted versus 1/BRAD (d) in Fig. 2 to enhance the visualization. Notably, when the values for $WFPS_{thresh}$ were below 45 %, methane emission rates increased, but BRAD had no influence on the emission rates. In instances where $WFPS_{thresh}$ values exceeded 90 %, emission rates were minimal, and BRAD no longer exerted a distinct influence on methane emission rates under AWD conditions. Consequently, our findings support the significance of BRAD in predicting methane emissions under conditions where soil water content ranges from 50 % to 90 % of the soil pores. Most importantly, methane emissions were highest whenever $WFPS_{thresh}$ was greater than 45 %.

To select the best parameters, we conducted a comparative analysis between simulated daily CH_4 values and measured data, resulting in a D-Statistic ranging from 0.12 to 0.91 and an RMSE between 0.23 and 1.44 kg[C] $ha^{-1}d^{-1}$across four crop seasons, depending on the variation in $WFPS_{thresh}$ and BRAD. For each $WFPS_{thresh}$ and BRAD combination, the average D-Statistic values ranged between 0.39 and 0.77, while RMSE ranged between 0.42 and 1.03 kg[C] $ha^{-1}d^{-1}$. In our selection process, we prioritized parameter combinations with higher D-Statistic values, leading to nine combinations with a D-Statistic of 0.77. From these options, we selected parameter combinations with the lowest RMSE. Further refinement involved selecting combinations with the lowest standard deviation among the cropping seasons for both D-Statistic and RMSE. Our analysis identified that, on average, $WFPS_{thresh}$ = 70 % combined with BRAD = 0.070 d^{-1} exhibited the best performance for the BRS Pampa cultivar conducted in Capão do Leão.

3.2. Simulation of crop phenology, final aboveground biomass, and grain yield

We calibrated CERES-Rice using experimental data from field experiments conducted in Capão do Leão. After final calibration, the model demonstrated correctly simulated values for the R4 and R9 stages (Counce et al., 2000) across all cultivars under continuous flooding conditions for the S3 cropping season (Fig. 3A). The crop cycle (time between planting to physiological maturity) ranged from 117 to 154 days among the cultivars that were used in this study, showing A705 as a shorter cycle and XP 113 as a longer cycle cultivar. The experimental plots under AWD conditions did not have phenology documented and were, therefore, not included in the analysis. The predictive capability of the model (S1, S2, and S4) showed that the bias between measured and observed values varied in absolute terms from 0 to 12 days for R4 and from 0 to 18 days for R9 (Fig. 3A).

In the calibration process for BRS Pampa, BRS Pampeira, A705, and XP 113 under continuous flooding conditions for the S3 season, the target was to minimize the difference between simulated and measured data for aboveground biomass (Fig. 3B) and grain yield (Fig. 3C). During the calibration of cultivars, bias (absolute values) ranged from 12 to 1591 kg ha^{-1} for aboveground biomass and 0–802 kg ha^{-1} for grain yield. Cultivar A705 exhibited the best performance for the simulation of grain yield, while XP 113 showed the best performance for aboveground biomass. In evaluating CERES-Rice performance, we observed aboveground biomass and grain yield, with values close to the 1:1 line of equality. The absolute average bias across cropping seasons, cultivars, and irrigation practices used in the model evaluation was 663 kg ha^{-1} (3.94 %) for aboveground biomass and 753 kg ha^{-1} (6.84 %) for grain yield. Our findings exhibit consistency with previous studies that used CERES-Rice. Dass et al. (2012) reported a bias in grain yield of 4.34 % for the Dhan 4 cultivar and 11.4 % for Hybrid 644, based on experiments conducted under AWD conditions in India. Similarly, Alejo (2021) compared simulated grain yield with field data for the NSIC Rc 192 cultivar in the Philippines, revealing a bias of 11.17 % under rainfed conditions, supplemented with irrigation when rice exhibited signs of

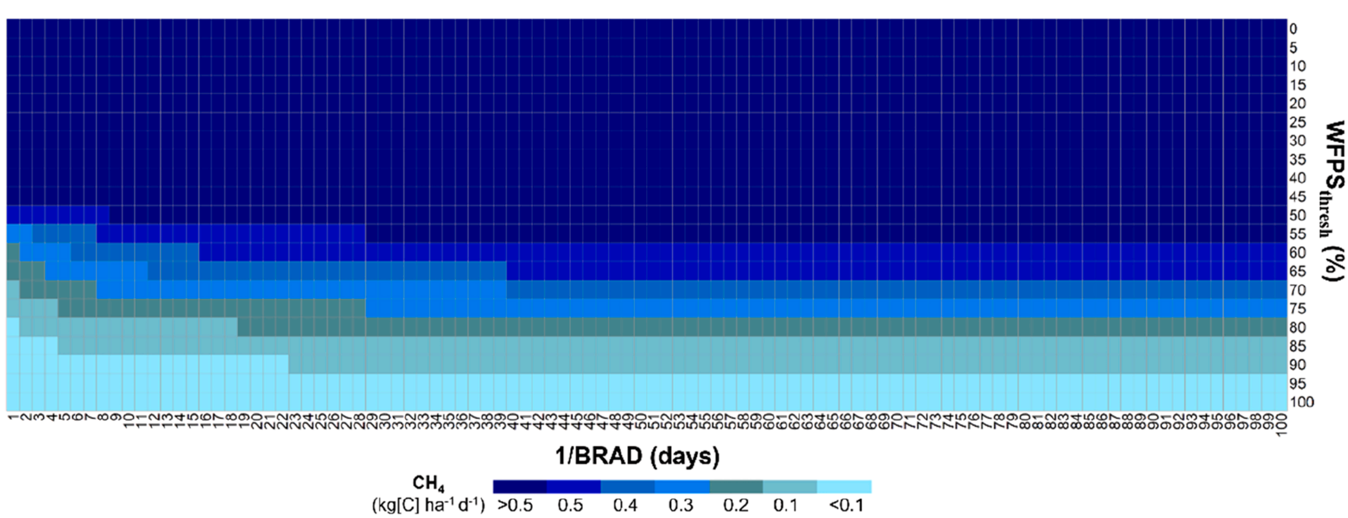

Fig. 2. Sensitivity analysis under alternate wetting and drying irrigation practices for the BRS Pampa cultivar over four cropping seasons (2019–2023) for daily methane (CH_4) emissions as a function of the variation of the fraction of water-filled porosity above which methane production occurs ($WFPS_{thresh}$) and soil buffer regeneration rate after drainage (BRAD). Averaged daily CH_4 (kg[C] $ha^{-1}d^{-1}$) emission values are represented by a blue gradient.

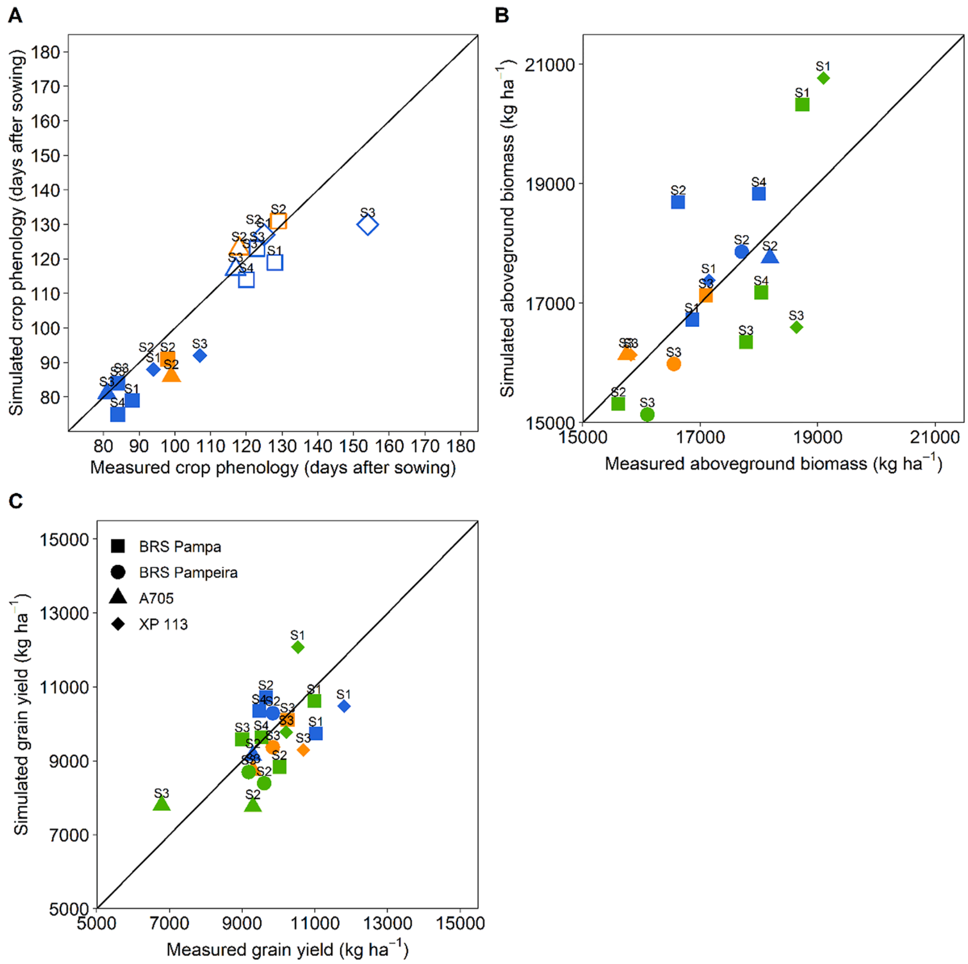

Fig. 3. Simulated and measured crop phenology (A), aboveground biomass (B), and grain yield (C) for rice cultivars BRS Pampa, BRS Pampeira, A705, and XP113, under two irrigation practices: continuous flooding (orange symbols representing experiments used for model calibration, and blue symbols representing experiments used for model evaluation) or alternate wetting and drying (green symbols), over four crop seasons (S1 – 2019/2020, S2 – 2020/2021, S3 – 2021/2022, S4 – 2022/2023) in Capão do Leão. In plot A, full symbols represent the anthesis date (R4), and empty symbols represent the physiological maturity date (R9). The 1:1 line of equality is shown (black line).

wilting. Darikandeh et al. (2023) calibrated the Hashami cultivar and observed a bias of 16.8 % in grain yield for northern Iran under full irrigation.

3.3. Simulation of daily methane emissions under continuous flooding and alternate wetting and drying irrigation practices

We assessed the performance of the DSSAT-GHG module in simulating methane emissions from paddy rice under CF and AWD irrigation practices. Our investigation focused on four rice cultivars, BRS Pampa, BRS Pampeira, A705, and XP 113, under four consecutive cropping seasons. Notably, the model captured the tendency of CH_4 emissions over the seasons, rice cultivars, and water availability (Figs. 4, 5, 6, 7) for AWD conditions after changes in BRAD and $WFPS_{thresh}$ parameters. These adjustments enabled the model to effectively simulate methane emissions in paddy rice under non-flooded conditions. Prior to this modification, the model consistently simulated CH_4 emission values at zero, assuming flooding as a prerequisite for methane emissions. The DSSAT-GHG default module showed an average D-Statistic of 0.42 and a RMSE of 0.50 kg [C] $ha^{-1}d^{-1}$, whereas the calibrated module had a D-Statistic of 0.70 and a RMSE of 0.47 kg [C] ha^{-1}. These improvements align with field data provided in this study, as well as several experiments conducted worldwide that have documented methane emissions in paddy rice under AWD conditions (*e.g.*, Setyanto et al., 2018; Fertitta-Roberts et al., 2019; Sriphirom et al., 2019).

The adjustments of the parameters of the DSSAT-GHG module had a minimal effect on the model response for simulating CH_4 production under CF conditions. For the DSSAT-GHG default module, the average D-Statistic was 0.84, and the average RMSE was 1.08 kg [C] ha^{-1}, while the D-Statistic was 0.87 and the RMSE was 1.00 kg [C] ha^{-1} after the changes of the parameters. This result was expected, considering the crop was flooded for most of the time, resulting in $WFPS_{thresh}$ consistently at 100 %. Consequently, BRAD does not induce variation in simulated methane production under these conditions, as was demonstrated in the sensitivity analysis (Fig. 2). The subtle improvement in the model can be attributed to an adjustment in simulations at the beginning of the crop and after draining the paddy rice before harvesting.

The experiments conducted under CF and AWD conditions showed distinct daily methane production rates for the subtropical environment. The AWD condition was able to reduce the daily methane production rate from 0.98 to 0.19 [C] ha^{-1} for the simulated conditions and from 1.38 to 0.29 kg [C] ha^{-1} under field conditions, both when compared with CF conditions. After adjusting the $WFPS_{thresh}$ and BRAD parameters, the DSSAT-GHG module successfully simulated methane production for non-flooded conditions, aligning with values observed in field experiments; however, the model showed the tendency to underestimate daily methane emissions under both CF and AWD conditions. Simulated and measured daily methane emissions from paddy rice were consistently lower for CF than for AWD irrigation practices. Our findings align with other studies where methane emissions in AWD were reported to be

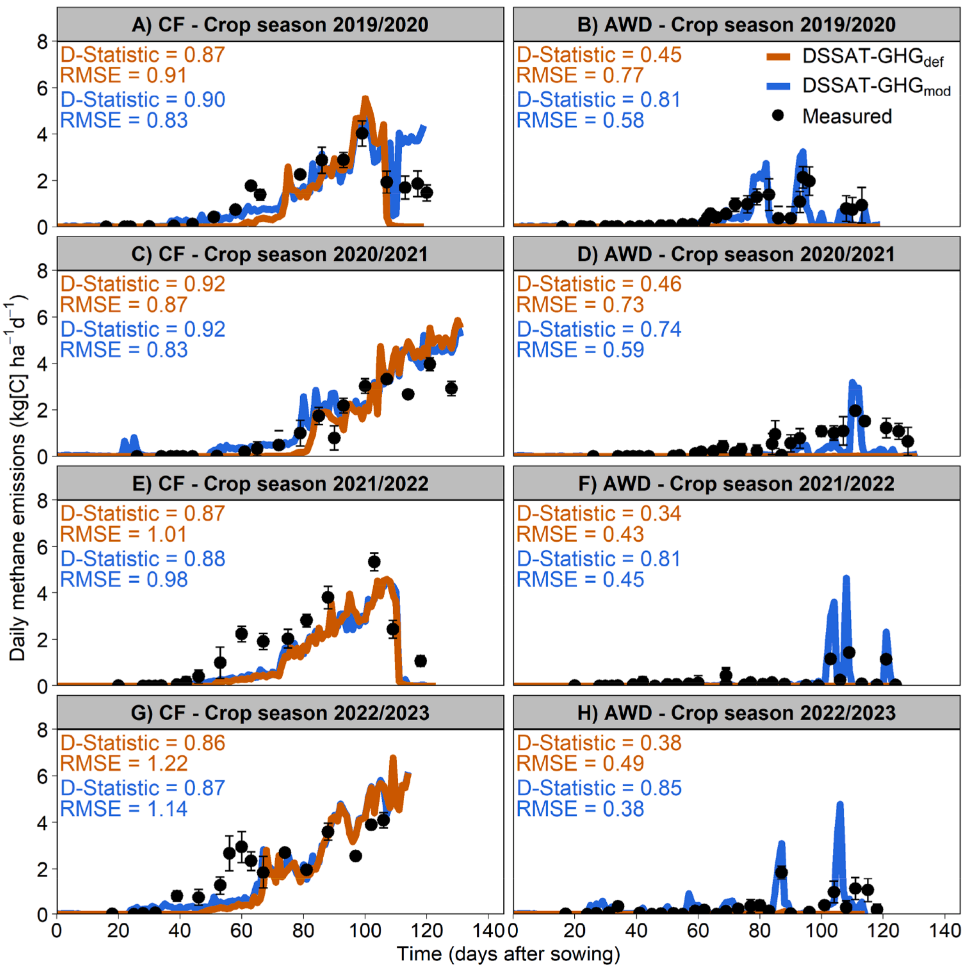

Fig. 4. DSSAT-GHG module simulations using default (def) or modified (mod) parameters and observed daily methane emissions for the BRS Pampa rice cultivar for continuous flooding (CF; A, C, E, G) and alternate wetting and drying (AWD; B, D, F, H) over four cropping seasons (2019–2023) in Capão do Leão. Error bars represent standard deviation.

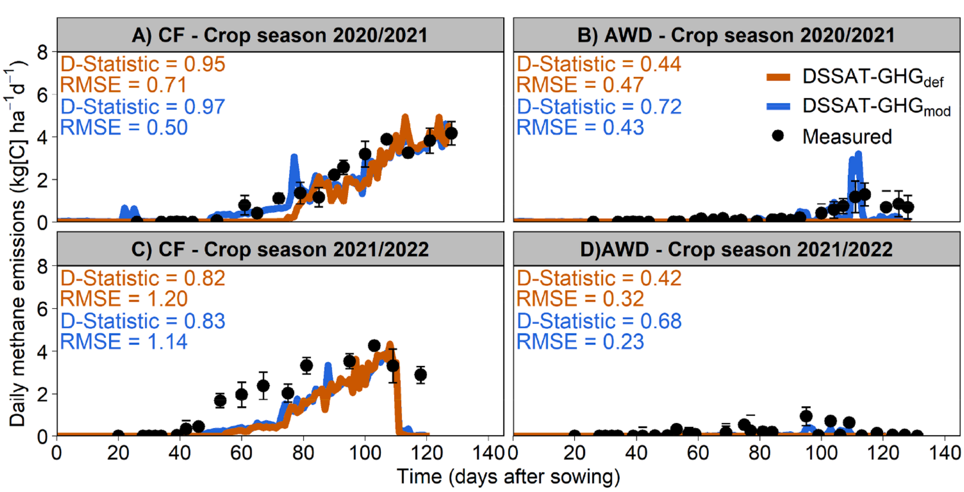

Fig. 5. DSSAT-GHG module simulations using default (def) or modified (mod) parameters and observed daily methane emissions for the BRS Pampeira rice cultivar for continuous flooding (CF; A, C) and alternate wetting and drying (AWD; B, D) over four cropping seasons (2019–2023) in Capão do Leão. Error bars represent standard deviation.

33–62 % lower than in CF conditions (Samoy-Pascual et al., 2019; Anapalli et al., 2023; Hoang et al., 2023).

We also assessed the response of all rice cultivars across each cropping season, focusing on comparing the response pattern of each rice cultivar to daily CH_4 emissions. During the S1 growing season, we noted higher CH_4 emission for the cultivar BRS Pampa than for XP 113 for both simulated and measured under CF conditions (Figs. 4 and 7). Under AWD conditions during the S2 growing season, the cultivars exhibited

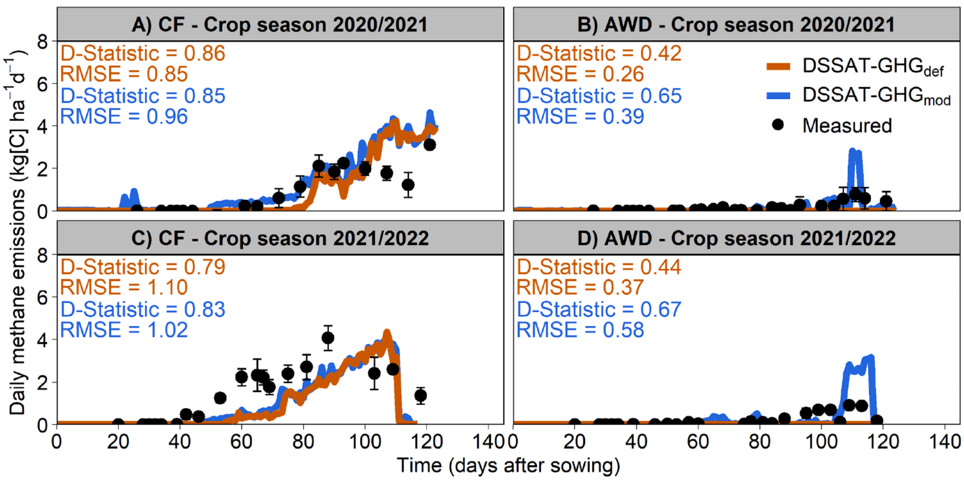

Fig. 6. DSSAT-GHG module simulations using default (def) or modified (mod) parameters and observed daily methane emissions for the A705 rice cultivar for continuous flooding (CF; A, C) and alternate wetting and drying (AWD; B, D) over four cropping seasons (2019–2023) in Capão do Leão. Error bars represent standard deviation.

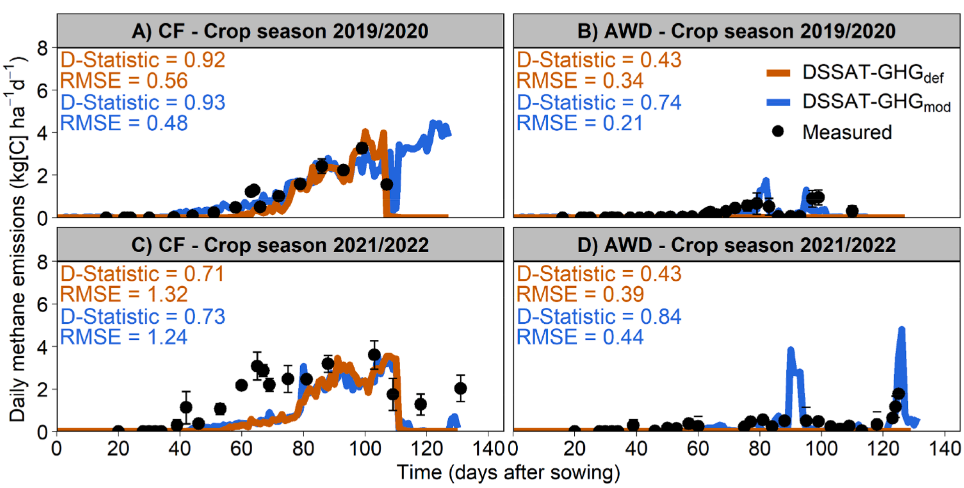

Fig. 7. DSSAT-GHG module simulations using default (def) or modified (mod) parameters and observed daily methane emissions for the XP 113 rice cultivar for continuous flooding (CF; A, C) and alternate wetting and drying (AWD; B, D) over four cropping seasons (2019–2023) in Capão do Leão. Error bars represent standard deviation.

similar simulated average daily CH_4 measured emissions (Figs. 4, 5, 6): 0.14 kg [C] ha^{-1} d^{-1} for both the cultivars BRS Pampa and BRS Pampeira, and 0.12 kg [C] ha^{-1} d^{-1} for the cultivar A705. During the S3 growing season under CF conditions, the average simulated values ranged from 0.89 to 1.22 kg [C] ha^{-1} d^{-1} while measured daily CH_4 emission ranged from 1.37 to 1.53 kg [C] ha^{-1} d^{-1} across all cultivars (Figs. 4,5,6,7), indicating a systematic underestimation by DSSAT-GHG module. During the S4 growing season, the cultivar BRS Pampa showed a higher average daily CH_4 emission at 1.67 kg [C] ha^{-1} d^{-1} (simulated) and 1.85 kg [C] ha^{-1} d^{-1} (measured) compared to the S1, S2, and S3 growing seasons. This increased CH_4 emission is likely associated with the higher average minimum (19.7ºC) and maximum (30.2ºC) temperatures during S4 (Supplementary Materials – Figs. S1–S4). It is important to note that elevated temperatures contribute to increased CH_4 emissions by enhancing the activity of methanogens (Chun et al., 2016; Lee et al., 2023).

The emission patterns of methane across different rice cultivars, as observed for both the simulated and measured values, exhibited variation. Given the cultivars that were used in this study and the subtropical environment, it appears challenging to establish a clear condition where one cultivar consistently emits either more or less methane than another. Therefore, selecting specific cultivars within this studied context is not a practical strategy for reducing CH_4 emissions. However, some studies suggest that depending on the rice cultivar, methane emissions can vary by up to 50 % (Hu et al., 2023; Lee et al., 2023). One possible explanation for the variation in methane emissions among rice cultivars is related to carbon allocation. Cultivars that emit less methane allocate more carbon to aboveground tissues. This allocation reduces the amount of organic carbon available for methanogenesis (Liu et al., 2017).

Although this study evaluated methane emissions over four growing seasons and five rice cultivars under two irrigation systems, a key limitation is that the simulations were conducted in a single environment and soil type. This could restrict the generalizability of the model's findings to other climates and soil conditions. Future applications of this tool should account for these limitations, and additional testing across diverse environmental settings is necessary to ensure broader applicability and robustness of the model's performance.

3.4. Long-term simulations of irrigation practices, grain yield, and methane emissions for paddy rice under a subtropical environment

Following the evaluation of the CERES-Rice model for the simulation of grain yield and the DSSAT-GHG module for CH_4 emissions, we conducted a scenario analysis of different irrigation practices. The results for the long-term simulations of paddy rice as a function of different irrigation practices for 30 years of historical weather data in Capão do Leão are presented in Fig. 8. The simulated grain yield ranged from 10,207 to 12,897 kg ha^{-1}, the average grain yield was lower 10,207 kg ha^{-1} for CF and was higher 11,251 kg ha^{-1} under S-50 % irrigation practice (Fig. 8A). The slightly higher grain yield observed in S-50 % can be attributed to greater nitrogen availability. The model simulated higher nitrogen losses under irrigation practices requiring more water.

As expected, the largest amount of seasonal applied irrigation (Fig. 8B) resulted in the highest amount of cumulative methane emissions (Fig. 8C). For CF, the average accumulated methane emission was approximately 39.5 kg [C] ha^{-1} d^{-1}, with an average seasonal applied irrigation of 442 mm. These values were close to the S-90 % scenario, which had an average accumulated methane emission of around 38.1 kg [C] ha^{-1} d^{-1} and required 382 mm of seasonal applied irrigation. These similar CF and S-90 % results can be attributed to the soil conditions in Capão do Leão, characterized by poorly drained soil with a high clay content. This, in turn, influenced the simulated CH_4 emission values for sprinkler irrigation, mainly when triggered at 80–90 % soil water remaining, easily establishing conditions conducive to methane production ($WFPS_{thresh} > 70$ %). The S-50 % scenario presented the lowest average accumulated methane emission of 31.9 kg [C] ha^{-1} d^{-1} and a smaller average amount for seasonal irrigation of 442 mm.

The average CWMP values vary from 40 % to 66 % (Fig. 8D) among the different irrigation practices that were evaluated with these scenarios. The S-50 % scenario exhibited the highest CWMP, with an average of 52 %, making it the most sustainable option when comparing grain yield, seasonal irrigation applied, and methane emissions. In contrast, the CF treatment proved the least viable due to its lower CWMP, higher methane emission values, increased water demand, and lower grain yield. These findings emphasize the importance of considering the intricate balance between rice grain yield, water use, and methane emission mitigation when evaluating the sustainability of various irrigation practice scenarios. A higher CWMP index indicates more efficient rice production in relation to each unit of water used and methane emitted. Among the long-term simulations that were analyzed in this study, environmentally conscious irrigation practices were best exemplified by the sprinkler system with irrigation triggered at 50 % soil water remaining.

Although these findings are based on simulations conducted for a specific location in a subtropical environment, they offer valuable insights into the broader environmental implications of irrigation practices. Reducing methane emissions from rice paddies is critical for global efforts to mitigate climate change, as methane is a potent greenhouse gas. Our results suggest that irrigation strategies, such as the S-50 %

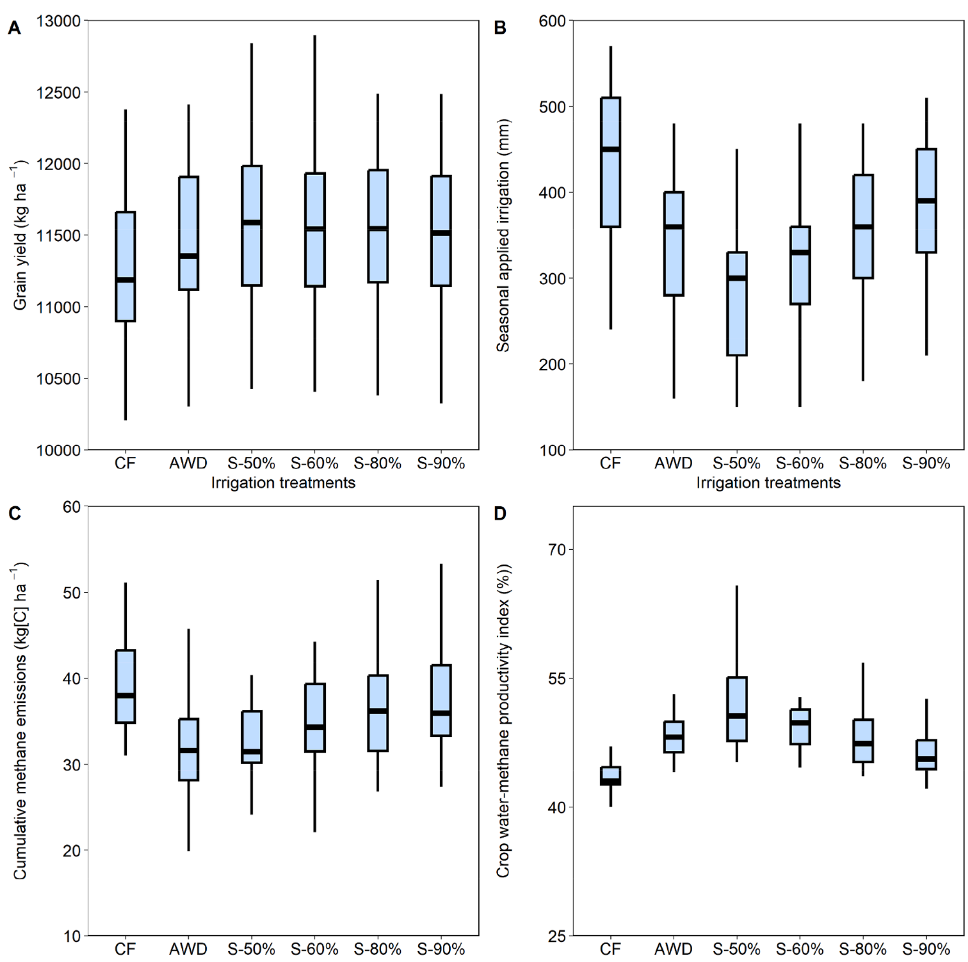

Fig. 8. Long-term simulations (1990–2019) for Capão do Leão under different irrigation practices scenarios: continuous flooding (CF), alternate wetting and drying (AWD), and sprinkler (S) with irrigation triggered at 50–90 % soil water remaining in the top 0.20 m of the soil profile. Boxplots represent the 10th, 25th (lower quartile), 50th (median), 75th (upper quartile), and 90th (upper whisker) percentiles.

scenario, could potentially balance methane reduction and rice yield in regions with similar environmental conditions. These results may contribute to global methane reduction efforts and support the implementation of climate-smart agriculture. However, it is important to note that further research is needed to confirm these trends in other regions with different environmental and soil characteristics.

Understanding the mechanisms of methane production is a central focus of current scientific exploration. To enhance the precision of the model in replicating diverse conditions that influence methane emissions, it is crucial to conduct additional evaluations under varying weather conditions, soil textures, and crop systems. Methane production, which typically occurs in anaerobic environments, exhibits reduced activity in the presence of oxygen, though not entirely inactive. This is particularly evident under conditions of partially saturated soil or in anaerobic microsites within the soil, as well as in methane production within plant tissue under aerobic conditions (Keppler et al., 2009; Kartal et al., 2013; Roth et al., 2023). We also suggest allocating BRAD and $WFPS_{thresh}$ parameters to an external model input file, enabling users to adjust them based on their soil type, irrigation, or environmental conditions. Furthermore, future studies could consider more in-depth research on the impact of climate change on GHG emissions using the DSSAT, which has proven to be a valuable tool for analyzing the effect of future climate scenarios on agricultural systems (Figueiredo Moura da Silva et al., 2021; Antolin et al., 2021).

4. Conclusion

Sensitivity analysis revealed that the original DSSAT-GHG module with default parameters only simulated methane emissions under flooded conditions. Therefore, we made modifications to the source code for soil-related parameters. After implementing these changes, we were able to successfully simulate daily methane emissions under alternate wetting and drying irrigation practices. There was a good agreement between simulated and measured crop phenology, grain yield, aboveground biomass, and daily methane emissions under different irrigation practices. Long-term simulations demonstrated that the amount of irrigation water and methane emissions for rice grown in a subtropical environment could be reduced while maintaining a high grain yield levels using sprinkler practices triggered at 50 % soil water remaining. In conclusion, the model accurately simulated rice grain yield and daily methane emissions for a subtropical environment, demonstrating that DSSAT can be applied to evaluate various irrigation management options to help conserve water use and reduce methane emissions in paddy rice.

CRediT authorship contribution statement

Gerrit Hoogenboom: Writing – review & editing, Visualization, Supervision. **Evandro H. Figueiredo Moura da Silva:** Writing – review & editing, Writing – original draft, Visualization, Validation, Resources, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Silvio Steinmetz:** Data curation. **Carlos E. Pellegrino Cerri:** Writing – review & editing, Visualization, Supervision, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Kenneth J Boote:** Writing – review & editing, Visualization, Supervision. **Santiago Vianna Cuadra:** Writing – review & editing, Validation, Investigation, Formal analysis, Data curation, Conceptualization. **Cheryl H Porter:** Writing – review & editing, Visualization, Investigation. **Walkyria Bueno Scivittaro:** Writing – review & editing, Data curation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.agwat.2024.109234.

Data Availability

Data will be made available on request.

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