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Daycent Simulation of Methane Emissions, Grain Yield, and Soil Organic Carbon in a Subtropical Paddy Rice System

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ABSTRACT: The DayCent ecosystem model, widely tested in upland agroecosystems, was recently updated to simulate waterlogged soils. We evaluated the new version in a paddy rice experiment in Southern Brazil. DayCent was used to simulate rice yield, soil organic carbon (SOC), and soil CH_4 fluxes. Model calibration was conducted with a multiple-year dataset from the conventional tillage treatment, followed by a validation phase with data from the no-tillage treatment. Model performance was assessed with statistics commonly used in modeling studies: root mean square error (RMSE), model efficiency (EF), and mean difference (M). In general, DayCent slightly underestimated rice yields under no-tillage (by 0.07 Mg ha^{-1}, or 9.2 %) and slightly overestimated soil C stocks, especially in the first years of the experiment. A comparison of observed and simulated CH_4 daily fluxes showed that DayCent could simulate the general patterns of soil CH_4 fluxes with slight discrepancies. Daily soil CH_4 fluxes were overestimated by 0.43 kg ha^{-1} day^{-1} (12 %). Growth-season CH_4 emissions under no-tillage were also somewhat overestimated (11 % or 45.29 kg ha^{-1}). We conclude that DayCent simulated SOC, rice yield, and CH_4 with some inaccuracies, but the overall performance was considered adequate. However, the model failed to represent the observed potential of no-tillage to mitigate CH_4 emissions, possibly because model algorithms could not capture the actual field conditions derived from no-tillage management, such as soil redox potential, plant senescence, and surface placement of plant residue.

Keywords: modeling, soil potential redox, flooded soil, greenhouse gas, soil tillage.

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INTRODUCTION

Rice is a major crop in southern Brazil, where the state of Rio Grande do Sul leads the country in cropped area (approximately 1.1 million ha) and yields (Conab, 2017). For many years, soil management for flooded rice production included deep tillage with moldboard or disc plows followed by multiple harrow operations to obtain a level seeding surface. More recently, however, research and technical assistance have helped to develop and introduce the no-tillage system in southern Brazil rice fields with a view to increasing soil quality, reducing operating costs, and optimizing seeding schedules (Sosbai, 2016).

Soil organic matter (SOM) dynamics in flooded production systems, which is associated with CH_4 fluxes, is a crucial factor for sustainable flooded rice production. In this anoxic soil environment, physical protection of SOM in soil aggregates is less effective in stabilizing SOM than in aerobic soils, possibly by the effect of water decreasing aggregate stability during the flooded rice growing season (Nascimento et al., 2009). Consequently, SOC is increased to a very small extent, if any, by the adoption of no-tillage in irrigated rice fields (Nascimento et al., 2009; Rosa et al., 2011; Ghimire et al., 2012; Das et al., 2014; Huang et al., 2016).

Flooded rice boosts CH_4 production and paddy rice fields are among the major sources of anthropogenic CH_4 released to the atmosphere (Le Mer and Roger, 2001). The global warming potential of CH_4 is roughly 28 times greater than that of CO_2; also, atmospheric CH_4 levels have risen by 150 % since 1750 (IPCC, 2013), with approximately 60 % of the global soil-to-atmosphere CH_4 emissions coming from anthropogenic sources (WMO, 2016).

Research conducted to assess soil CH_4 fluxes in southern Brazil has identified some strategies to mitigate soil CH_4 emissions in irrigated rice fields. Such strategies include no-tillage (Bayer et al., 2014), anticipated tillage (Bayer et al., 2015), and intermittent irrigation (Moterle et al., 2013; Zschornack et al., 2016), none of which decrease rice yields relative to traditional soil and water management practices. However, the high variability of soils, climate, and production systems encompassed by the 1.3 million ha of cropland in southern Brazil would make on-site quantification of CH_4 to assess site-specific variables a costly, labor-intensive task. In this context, simulation models provide useful research tools for expanding and integrating soil CH_4 emission estimation.

DayCent is a daily-step simulation model developed from the core algorithms of the well-known Century Soil Organic Matter model (Metherell et al., 1993). The model has been widely tested in upland soils (Plaza-Bonilla et al., 2014; Scheer et al., 2014; Congreves et al., 2015; Migliorati et al., 2015; Weiler et al., 2017). The model includes submodels for plant yield, crop residues and organic matter, soil water and temperature dynamics, and C and N gas fluxes. Plant yield is a function of genetic potential of the crop, nutrient availability, and soil moisture and temperature. Carbon and N are allocated to leaves, stems, and roots, and soil inflows are assumed to be controlled by the lignin-to-N ratio and by soil moisture, texture, and temperature. Organic carbon and nutrients in soil are divided into pools based on residence time, namely: active (0.5-1.0 yr), slow (10-50 yr), and passive (1,000-5,000 yr). Recently, a methanogenesis submodel was included in the original algorithms. Soil CH_4 fluxes in flooded rice paddies are assumed to be controlled by carbon substrate availability, plant growth, and soil redox potential and temperature. Early studies testing this expanded version showed adequate model performance in simulating trends in SOC content and CH_4 fluxes in agricultural regions of China (Cheng et al., 2013, 2014).

In this study, we assessed the ability of DayCent to simulate SOC, grain yield, and daily and seasonal soil CH_4 emissions in a subtropical rice cropping system in southern Brazil using data from a long-term field experiment.

MATERIALS AND METHODS

Experimental site

This study was conducted using data from a long-term field experiment established at the Rice Research Station of the *Instituto Riograndense do Arroz* - IRGA (Rice Institute of Rio Grande do Sul) in the municipality of Cachoeirinha (29.9° S; 51.1° W), Rio Grande do Sul, Brazil in 1994. The soils at this site are Gleysols (*Gleissolo Háplico*). The climate is humid subtropical (*Cfa*) according to the updated Köppen-Geiger classification system (Peel et al., 2007), characterized by warm summers (mean temperature 25 °C), cool winters (average 15 °C), and mean annual rainfall of 1,350 mm evenly distributed throughout the year.

Field experiment

The experiment was set up to investigate rice yields under contrasting soil tillage systems - conventional tillage and no-tillage - arranged in a randomized block design with three replicates. The cropping system was paddy rice as a summer crop and self-seeding ryegrass (*Lolium multiflorum* L.) as a cover crop without irrigation during the winter months. The conventional tillage treatment involved disking and two disk harrow operations in the spring prior to rice planting. In the no-tillage treatment, the ryegrass cover crop was desiccated with a glyphosate-based herbicide in the spring. After that, the standing biomass was chopped and rice was planted through the crop residues by using a no-till seed drill. In the rice season, experimental plots (28 × 40 m) were flooded approximately 20 days after planting and kept flooded under a 0.10-m water layer until about ten days before harvest. The soil and crop management schedules used are presented in table 1. Additional details regarding this experiment can be found in Bayer et al. (2014).

Table 1. Management practices in the rice growing seasons

Management	Season								
	2002/03[1]	2003/04[1]	2004/05	2005/06	2006/07	2007/08[1]	2008/09	2009/10[1]	2011/12[1]
Ryegrass biomass	Oct 18	Sep 30		Sep 22	Sep 27	Sep 12	Sep 16	Aug 31	Oct 15
Baseline N (kg ha^{-1})	Dec 10 (10)[2]	Nov 8 (15)	Nov 20 (15)	Nov 3 (15)	Oct 10 (20)	Oct 25	Nov 23 (20)	Oct 24 (15)	Oct 15
Rice seeding	Dec 10	Nov 8	Nov 20	Nov 3	Oct 10	Oct 25 (20)	Nov 23	Oct 24	Oct 15 (20)
Soil flooding	Dec 30	Dec 2	Dec 14	Nov 29	Nov 9	Nov 16	Dec 14	Nov 18	Nov 11
N fertilization (kg ha^{-1})	Dec 30 (50)	Dec 2 (55)	Dec 14 (80)	Nov 29 (80)	Nov 9 (80)	Nov 16 (67)	Dec 14 (100)	Nov 18 (100)	Nov 11 (100)
N fertilization (kg ha^{-1})	Jan 31 (40)	Dec 29 (25)	Jan 14 (40)	Jan 6 (40)	Dec 12 (40)	Dec 19 (33)	Jan 14 (50)	Dec 21 (40)	Dec 7 (50)
N fertilization (kg ha^{-1})	Feb 19 (30)	Jan 5 (50)	-	-	-	-	-	-	-
Soil drainage	Apr 1	Mar 8	Feb 21	Feb 21	Jan 30	Feb 18	Feb 22	Feb 19	Feb 6
Harvest	Apr 5	Mar 23	Mar 28	Mar 10	Feb 14	Mar 5	Mar 27	Mar 1	Feb 16

[1] Rice growing systems reported by Bayer et al. (2014). [2] The values in brackets mean applied nitrogen rates. - = no fertilizer-N application.

Experimental dataset

Plant, soil, and greenhouse data were obtained from previous studies conducted in the same experiment (Bayer et al., 2014). Grain yield was determined with a plot harvester in the nine rice-growing seasons from 2002 to 2012 (9th to 19th year of the experiment). Yields for 2002/2003, 2003/2004, 2007/2008, 2009/2010, and 2011/2012 have already been reported by Bayer et al. (2014). Baseline SOC data were obtained from Costa (2005) and Nascimento et al. (2009). Additionally, a soil sampling survey was conducted in 2015 to expand the SOC dataset under both tillage systems. Soil samples were obtained from the 0.00-0.20 m soil layer, and soil carbon content was determined by dry combustion on a Shimadzu TOC-VCSH analyzer. Carbon stocks were estimated as equivalent soil mass, taking the soil under conventional tillage as a reference. Additional input data for the DayCent model, such as soil hydrological and physical properties for this soil class (Gleysol), were obtained from Uhde (2009).

Daily meteorological data for the 1964-1999 period were obtained from a weather station in Porto Alegre, 13 km from the experimental site, and data since 2000 from an automatic weather station at the research station.

Daily soil CH_4 fluxes, measured in five rice-growing seasons (2002/2003, 2003/2004, 2007/2008, 2009/2010, and 2011/2012), were evaluated by the static closed chamber method. Briefly, the chambers consisted of a 0.60 × 0.60 × 0.20 m aluminum top and an aluminum base of the same size. Chamber bases were driven 0.05 m deepth into the soil before permanent flooding and remained in it throughout the growing season. Each base had an open bottom and sealable channels on the sides to allow irrigation water to flow freely, the channels being sealed during air sampling events. Each base covered three rice plant rows. Additional, 0.20 or 0.30 m aluminum extensions were stacked on the bases as the rice plants grew taller, and the expanded chamber volume was used in greenhouse gas emission calculations. Air was drawn with polypropylene syringes, transferred to the Biogeochemistry Laboratory at UFRGS and analyzed for CH_4 concentration in a Shimadzu gas chromatograph. Daily CH_4 fluxes were calculated according to Bayer et al. (2014) and seasonal emissions by trapezoidal integration of daily fluxes throughout the growing seasons. Details regarding air sampling, analysis, and calculation of CH_4 fluxes and seasonal emissions are available in Bayer et al. (2014) and Zschornack et al. (2016).

Model initialization, calibration, and validation

A model spin-up simulation of 6,000 years using natural grassland under moderate grazing was conducted to initialize DayCent (Parton et al., 1987; Del Grosso et al., 2011). This initial step was followed by a baseline simulation of paddy rice cropping for 50 years, consistent with site historical records from the Rice Research Station.

Model calibration was conducted with SOC, rice grain yield, and soil CH_4 flux data from the conventional tillage treatments, and data from the no-tillage system were used to validate the model. The calibration step involved multiple model runs, inspecting output, and iterative modification of the default biomass production parameter PRDX(1) of rice and ryegrass in the CROP.100 file until SOMSC (SOC output variable) matched measured SOC stocks. Additional parameterization consisted of changes in the root parameter (FREXUD) that determine root C exudates, from default 0.45 to 0.60 (Cao et al., 1995).

Statistical tests

This modeling exercise was evaluated (both calibration and validation steps) using statistics commonly applied in this context (Smith et al., 1997): root mean square error (RMSE, Equation 1), model efficiency (EF, Equation 2), and mean difference (M, Equation 3), with a t-test used to assess significant differences in M (Equation 4). The equations used to calculate these statistics are the following:

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(Si\text{-}Oi)^2}{n}} \quad \text{Eq. 1}$$

$$EF = \frac{\sum_{i=1}^{n}(Oi\text{-}Si)^2}{\sum_{i=1}^{n}(Oi\text{-}\bar{O})^2} \quad \text{Eq. 2}$$

$$M = \sum_{i=1}^{n} \frac{(Si\text{-}Oi)}{n} \quad \text{Eq. 3}$$

$$t = \frac{M \times \sqrt{n}}{\sqrt{\sum_{i=1}^{n}[(Oi\text{-}Si)\text{-}M]^2/(n\text{-}1)}} \quad \text{Eq. 4}$$

in which *Oi* denotes the observed and *Si* simulated values; $\bar{O}$ is the mean of the observed data; and *n* is the number of measurements. Positive M values indicate that the model underestimated the observed values, whereas negative M values indicate overestimation. If the t-value is greater than the critical two-tailed 2.5 % t-value, the simulations have a significant positive or negative bias (depending on the M calculated). In addition, observed and simulated data from conventional tillage and no-tillage were visually compared in plots highlighting 1:1 lines.

RESULTS AND DISCUSSION

Calibration

The iterative calibration procedure improved DayCent performance in this southern Brazilian paddy rice system, assessed by statistical tests on simulated and measured rice yield, SOC, and CH_4 fluxes (Table 2), in comparison to initial runs with the default parameters.

Validation

In the following section we present and discuss simulation of the no-tillage treatment that was used to validate application of the model in paddy rice systems in southern Brazil.

Rice yields

Simulated rice yields under no-tillage were compared with observed data (Figures 1 and 2). DayCent slightly underestimated rice yields, by 0.07 Mg ha^{-1} yr^{-1} (9.2 %) on average, without significant bias (Table 3). Similar studies in China were also able to simulate yield adequately (Stehfest et al., 2007; Cheng et al., 2013). As the efficiency statistics indicated acceptable performance, the results suggest that DayCent can accurately estimate rice yield in flooded soils in southern Brazil. Accurate simulation of plant biomass is crucial to estimate soil CH_4 emissions because carbohydrate exudation from roots, the major labile C source driving CH_4 emissions, is closely related to rice biomass (Cao et al., 1995; Cheng et al., 2013).

Table 2. Statistical analysis of simulated and observed parameters under conventional tillage treatment (model calibration) in a long-term experiment at the Rice Research Station in southern Brazil

Statistics	Calibration parameters			
	Rice yield	SOC	Daily CH_4 flux	Seasonal CH_4 flux
	Mg ha^{-1}		kg ha^{-1}	
RMSE	0.67	4.38	3.21	96.59
M	0.35	-2.34	0.47	48.13
t-test	ns	ns	ns	ns
		(-∞ to 1)		
EF	0.37	-0.13	0.09	-0.25

ns = non-significant (p<0.05). RMSE = root mean square error; M = mean difference; EF = model efficiency.

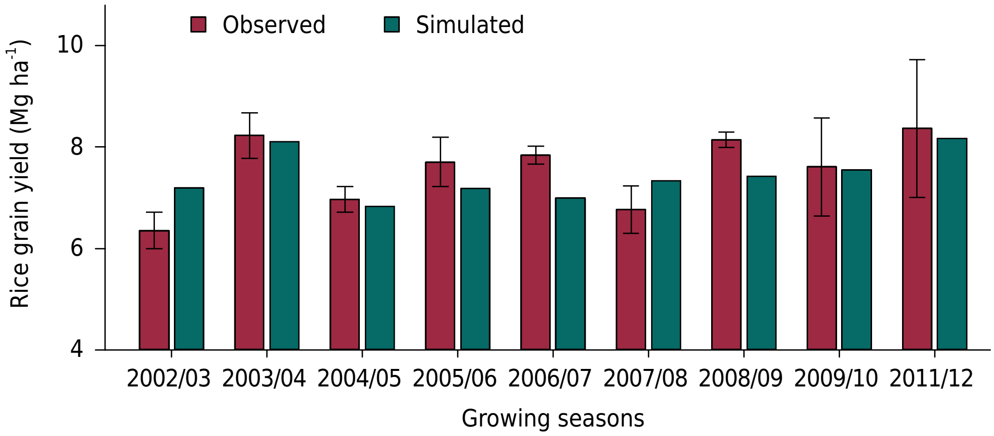

Figure 1. Observed and simulated rice grain yields under a no-tillage system in a long-term experiment in southern Brazil. Error bars represent standard deviations.

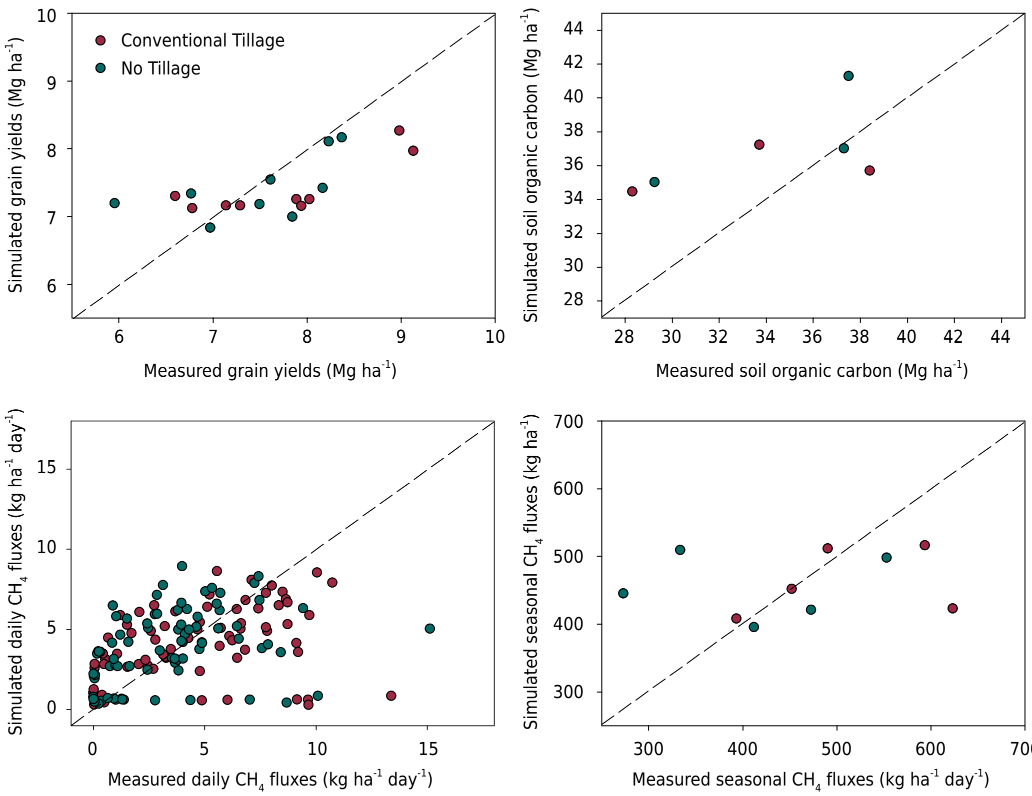

Figure 2. Comparison of observed and simulated rice grain yields, soil carbon, daily CH_4 fluxes, and seasonal CH_4 emissions under conventional and no-tillage.

Table 3. Statistical analysis of simulated and observed parameters under no-tillage treatment (model validation) in a long-term experiment at the Rice Research Station in southern Brazil

Statistics	Validation parameters			
	Rice Yield	Soil Carbon	Daily CH_4 flux	Seasonal CH_4 flux
	Mg ha^{-1}		kg ha^{-1}	
RMSE	0.60	3.99	3.00	115.45
M	0.07	-3.10	-0.43	-45.29
t-test	ns	ns	ns	ns
	(-∞ to 1)			
EF	0.35	-0.08	-0.06	-0.34

ns = non-significant (p<0.05). RMSE = root mean square error; M = mean difference; EF = model efficiency.

Soil organic carbon

Soil organic carbon stocks measured under the no-tillage treatment increased from 24 to 36 Mg ha^{-1} in 12 years, whereas the simulated SOC stocks increased from 36.7 to 42.2 Mg ha^{-1} (Figure 3). DayCent overestimated soil C stocks especially in the first years of the experiment (Table 3). The current SOC stocks observed (2015) corroborate what has been observed in previous studies on tillage systems in paddy rice: an increase in SOC in the topsoil, without significant differences across tillage systems (Nascimento et al., 2009; Cheng-Fang et al., 2012; Huang et al., 2016). Excess water in rice paddies may decrease physical protection of organic matter in soil aggregates in no-tilled flooded soils (Nascimento et al., 2009).

Earlier studies have shown that Century and DayCent were able to successfully model SOC in flooded environments (Chimner et al., 2002; Cheng et al., 2014). Cheng et al. (2014) was not able to adequately simulate SOC changes in Chinese rice paddies, most likely due to uncertainties in the experimental dataset (e.g., incomplete management history). This difficulty also applies to our study: model calibration could be much improved with detailed soil use and management information predating the 1990s. In any case, DayCent is more sensitive to recent management, so the absence of longer-term historical data on land use and management at the experiment site is not critical to model crop yield (as shown above) and soil CH_4 emissions (Del Grosso et al., 2011), which is the most important objective of this research effort.

Methane fluxes

A comparison of observed and simulated soil CH_4 daily fluxes showed DayCent to effectively simulate the general patterns of soil CH_4 fluxes, with only slight discrepancies (Figure 4). The model overestimated soil CH_4 daily fluxes by 0.43 kg ha^{-1} day^{-1} (12 %) under no-tillage, without significant bias (Table 3). It is noteworthy that the simulated soil CH_4 fluxes under no-tillage followed almost identical trajectories in comparison with simulated soil CH_4 fluxes under conventional tillage (data not shown). It has been reported that flooded rice systems under no-tillage have lower CH_4 emissions (Bayer et al., 2014). The differences between observed and simulated daily soil CH_4 fluxes were especially marked in three of the five rice growing seasons (2007/2008, 2009/2010, and 2011/2012), when the model failed to capture the observed increase in soil CH_4 emissions (Figure 4). This underperformance of the model in reproducing expected lower soil CH_4 fluxes under no-tillage might be explained by a combination of effects related to plant senescence, and soil redox potential which might have impaired DayCent performance at the end of the growing season, as we discuss below.

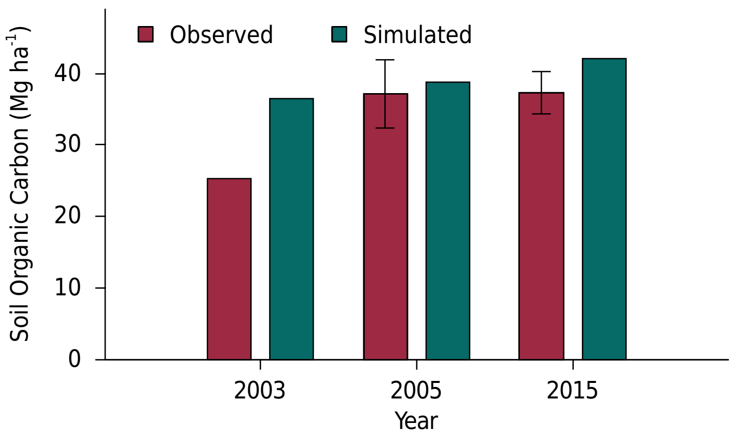

Figure 3. Observed and simulated soil organic carbon (SOC) from flood irrigated rice under a no-tillage system in a long-term experiment in southern Brazil. Error bars represent standard deviations.

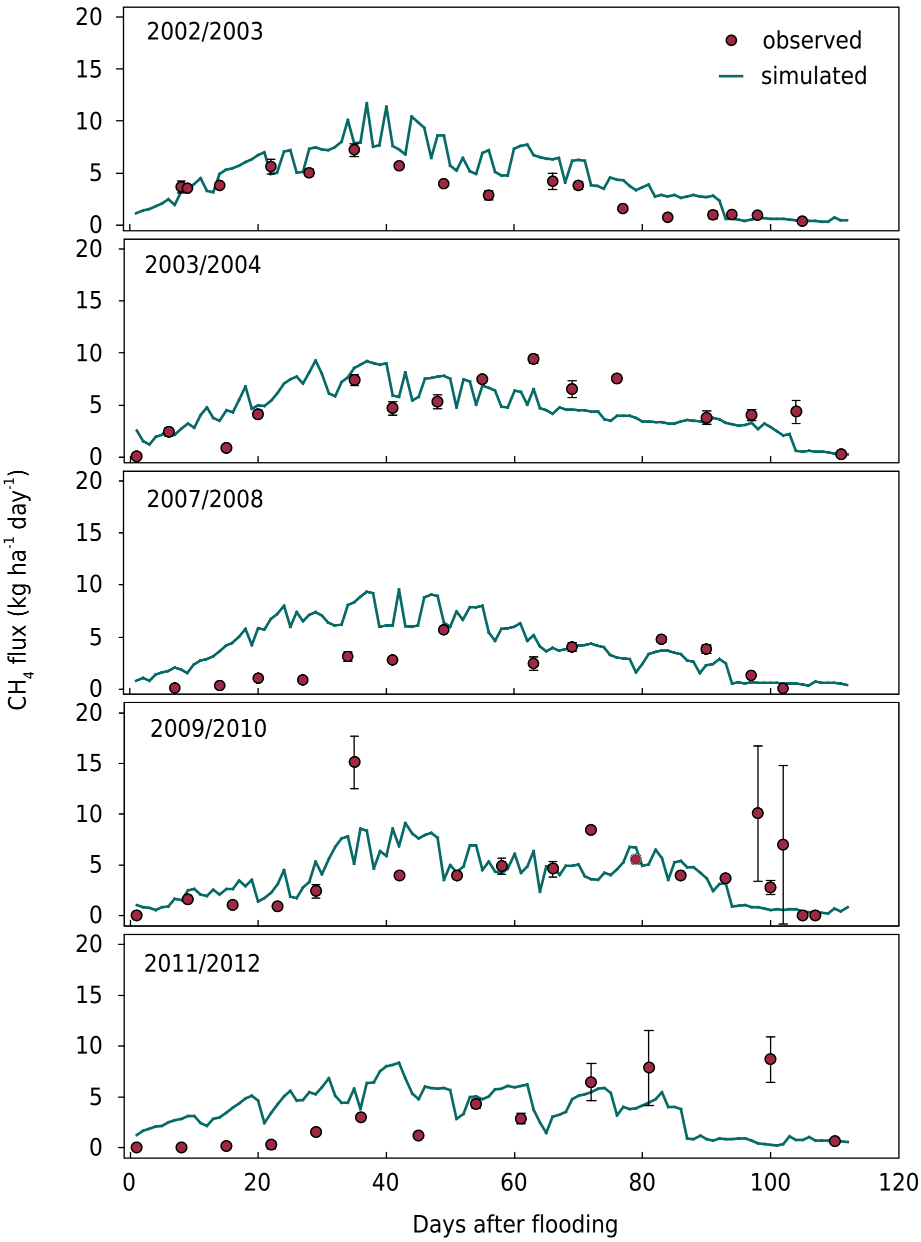

Figure 4. Simulated and observed daily soil methane (CH_4) fluxes in paddy fields under a no-tillage system in a long-term experiment in southern Brazil. Error bars represent standard deviations.

According to Bayer et al. (2014), increased C inputs from root exfoliation and plant senescence may cause CH_4 emissions to peak at the end of the growing season. DayCent includes parameters to determine root death rate under water stress conditions and shoot fractions dying during plant senescence; however, it does not allow one to assess C-root additions at the end of the rice life cycle. Also, soil redox potential at the end of the growing season may have been inaccurately represented by the model. Thus, the function used to simulate irrigation suppression and establish soil saturation controlled by rainfall and irrigation (FLOD 1) estimated an immediate change in redox potential from -250 to -20 mV. However, rainfall events at the end of the rice growing season in the above-mentioned years may have caused soil redox potential to remain in the negative region and enhanced CH_4 production in combination with greater root C exudation. Also, as suggested by Bayer et al. (2014), the high soil CH_4 fluxes observed after soil drainage may have resulted from the release of gas previously trapped in inundated soil, which was not accurately simulated by DayCent.

When growing-season CH_4 emissions were evaluated (Figures 5 and 2), the model also overestimated emissions (11.0 %, or 45.29 kg ha^{-1}), with no significant bias (Table 3), mostly due to large mismatches of CH_4 emissions in two growing seasons (2002/2003 and 2007/2008). In the other three seasons, the simulations were quite accurate in comparison with the observed values. Thus, DayCent was unable to represent the 21 % reduction in soil CH_4 emissions under no-tillage previously reported by Bayer et al. (2014) in the same experiment. Only a 2 % mitigation of CH_4 emissions from no-tillage in this 5-year period was simulated. In a meta-analysis of CH_4 emissions in Chinese rice fields, Feng et al. (2013) also reported that no-tillage could reduce CH_4 emissions by 26 % in comparison to conventional tillage. Li et al. (2011) attributed the lower CH_4 emissions in no-tillage system to higher soil bulk density and lower dissolved organic carbon content, which could restrict substrate availability for methanogenesis. We analyzed DayCent output and noted that it correctly simulated higher readily-decomposable C (METABC output variable) in conventional tillage treatments but only small differences in CH_4 emissions between soil tillage systems. This suggests that another mechanism that could reduce CH_4 emissions under no-tillage may not be accurately represented by the model, and the inaccuracy may have resulted from the inability of the model to capture the influence of tillage systems on soil redox potential and of the location of labile C input by crop residues under no-tillage.

In general, DayCent estimated a more negative soil redox potential under no-tillage (output variables not shown), owing to the increase in SOC content associated with this system. However, Bayer et al. (2014) showed in a greenhouse study that the soil redox potential was lower when crop residues were mixed with soil than when they were left at the soil surface. Thus, incorporating crop residues into anaerobic subsurface soil layers under conventional tillage potentially increases methanogenic activity and leads to higher soil CH_4 emissions. With no-tillage, however, crop residues are kept on the soil surface, where O_2 diffusion from the atmosphere and rice aerenchym facilitates the formation of layers with an increased redox potential. Also, some field studies have exposed a depth gradient in soil redox potential (Liesack et al., 2000; Reddy and DeLaune, 2008; Zschornack et al., 2011) that is currently not simulated by DayCent. Further development of the redox potential algorithm of the model may lead to a better ability to capture these relationships.

Although the primary soil CH_4 mechanisms are well studied and quantified, only a few modeling studies have reported these processes in depth, and experimental measurements rarely distinguish between methanogenesis and methanotrophy (Xu et al., 2016). Thus, it is not always possible to identify the impact of a single factor on CH_4 fluxes. For instance, the redox status of soil affects both methanogenesis and methanotrophy, and field measurements of soil CH_4 fluxes reflect a dynamic equilibrium between these two

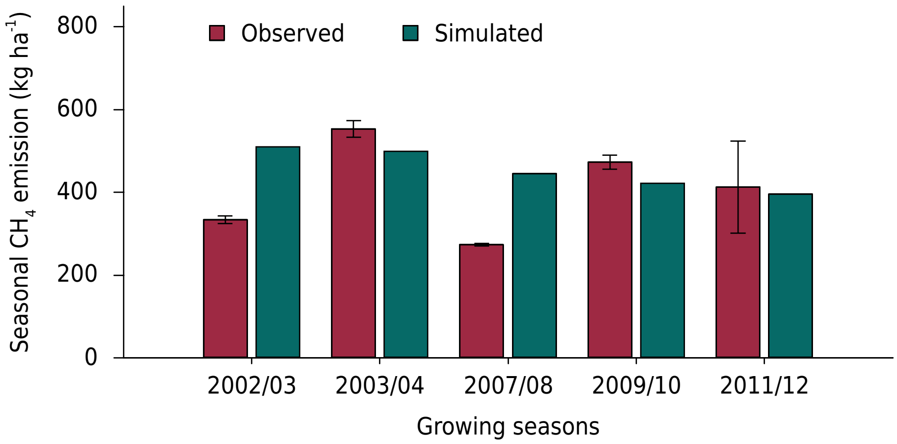

Figure 5. Observed and simulated seasonal soil methane (CH_4) emissions under a no-tillage system in a long-term experiment in southern Brazil. Error bars represent standard deviations.

processes. It is therefore impossible to ascertain whether DayCent tends to overestimate soil methanogenesis or underestimate methanotrophy under no-tillage.

CONCLUSIONS

The DayCent ecosystem simulated SOC, rice yield, and methane emissions in a southern Brazilian paddy rice field with some inaccuracies. The overall performance was considered adequate, as the CH_4 flux trajectories were adequately simulated. However, the model failed to represent the observed potential of no-tillage to mitigate soil CH_4 emissions, possibly because model algorithms were not able to capture the actual field conditions derived from no-tillage management, such as soil redox potential, plant senescence, and surface placement of plant residue.

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