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**Research article** 

# Parameterization, calibration and validation of the DNDC model for carbon dioxide, nitrous oxide and maize crop performance estimation in East Africa

ABSTRACT



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Dynamic biogeochemical models are crucial tools for simulating the complex interaction between soils, climate and plants; thus the need for improving understanding of nutrient cycling and reduction of greenhouse gases (GHG) from the environment. This study aimed to calibrate and validate the DeNitrification-DeComposition (DNDC) model for soil moisture, temperature, respiration, nitrous oxide and maize crop growth simulation in drier sub-humid parts of the central highlands of Kenya. We measured soil GHG fluxes from a maize field under four different soil fertility management practices for one year using static chambers and gas chromatography. Using experimental data collected from four management practices during GHG sampling period, we parameterized the DNDC model. The results indicate that the DNDC model simulates daily and annual soil moisture, soil temperature, soil respiration (CO<sub>2</sub>), nitrous oxide (N<sub>2</sub>O), N<sub>2</sub>O yield-scaled emissions (YSE), N<sub>2</sub>O emission factors (EFs) and maize crop growth with a high degree of fitness. However, the DNDC simulations slightly underestimated soil temperature (2-6%), crop growth (2-45%) and N<sub>2</sub>O emissions (5-23%). The simulation overestimated soil moisture (9-17%) and CO<sub>2</sub> emissions (3-10%). It however, perfectly simulated YSE and EFs. Compared to the observed/measured annual GHG trends, the simulation results were relatively good, with an almost perfect fitting of emission peaks during soil rewetting at the onset of rains, coinciding with soil fertilisation. These findings provide reliable information in selecting best farm management practice, which simultaneously improves agricultural productivity and reduces GHG emissions, thus permitting climate-smart agriculture. The good DNDC simulated YSE and EFs values (Tier III) provide cheaper and reliable ways of filling the huge GHG data gap, reducing uncertainties in national GHG inventories and result to efficient targeting of mitigation measures in sub-Saharan Africa.

# 1. Introduction

Climate change is principally a result of emissions of greenhouse gas (GHG), and which have been on the rise resulting to increased average global surface temperature (IPCC, 2014). The warming effects have been projected to potentially result to adverse climate-based issues such as low and erratic rainfall alongside prolonged drought conditions which in the long run results to a low agriculture production and food insecurity among the rain-fed agriculture smallholder farmers (Agovino et al., 2018). This calls for concerted efforts to address the needs of the ever increasing global population including food and general livelihoods improvement and a better understanding of the climate-related agricultural dynamics. More so, there is need for careful selection of sound cropland management practices which promotes soil carbon

sequestration, agricultural productivity and reduces GHG emissions, thus permitting climate-smart agriculture (Francaviglia et al., 2012).

Direct measurements of soil GHG fluxes for national inventories are almost impractical due to the high cost involved in quantification as it requires numerous measurements over large spatial and temporal extents (Giltrap et al., 2010). Thus, most developing countries cannot afford to establish these empirical studies and therefore rely heavily on default Tier I emission factors (EF) from the Intergovernmental Panel on Climate Change (IPCC) to report their nationally determined contributions (NDCs) as an obligation to the Paris Climate Agreement of 2015. According to Macharia et al. (2020) and Musafiri et al. (2020), agriculture-related Tier I emission factors tend to over-estimate GHG status in sub-Saharan Africa (SSA) leading to inflated national GHG inventories that may result in poor targeting of efficient adaptation and

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mitigation measures (Pelster et al., 2017). However, to overcome uncertainties in national GHG inventories, process-based models have been developed and which over time has been validated and found reliable to provide supplementary information on large spatial-temporal scales from areas with which it would have been too costly and impractical to acquire relevant information (Giltrap et al., 2010).

Dynamic biogeochemical models are essential tools for improving agricultural management and decision making (Guest et al., 2017). These models are great tools in deciphering the existing relationship between crop productivity and changing environmental and farm management practices (Lenz-Wiedemann et al., 2012) at the field, regional, national and global scales (Rui et al., 2017) and under different soil management technologies (Musafiri et al., 2021). More so, most of the process-based C and N cycling models simulate GHG emissions (Yue et al., 2019). Therefore, modelling of agroecosystems offers insight into C and N dynamics and provides an avenue for exploring practical mitigation measures (Giltrap et al., 2010). However, there is generally a scanty of information on the application of dynamic biogeochemical models for simulating soil GHG fluxes from different management practices for improvement of the existing inconsistencies in the national inventories in Kenya and SSA.

In this study, we used the DeNitrification-DeComposition (DNDC) model, which is one of the most utilized models for simulating crop growth as well as GHG emissions. The model has been put together to simulate various processes in agroecosystems' biogeochemistry (Yu et al., 2014). The model has had a global application in simulating crop production of major crops, such as maize (Musafiri et al., 2021), wheat and rice (Katayanagi et al., 2012) following application of different management practices, as well as simulating GHG fluxes (Rui et al., 2017; He et al., 2019). As such, this study aimed to achieve the following objectives; i) calibrate and validate the DNDC model, ii) simulate maize crop growth through carbon allocation along the crop components; leaves, stems, roots, and grains, and iii) evaluate the model's ability in simulating field-measured soil moisture, temperature, greenhouse gas emissions (CO2 and N2O), N2O emission factors (EFs) and N2O yield-scaled emissions (YSE) from four different fertiliser treatments in the central highlands of Kenya for a period of one year (February 2017 to February 2018).

# 2. Materials and methods

#### 2.1. Experimental site description

This study was conducted in Embu County, Kenya (00° 47' 26.8"S; 37° 39' 45.3"E). The trial was established in 2004 as described by Mucheru-Muna et al. (2010) which is located at an altitude of 1030 m a.s.l. The area experiences two rainfall seasons with the long rain (LR) season running from March to May while the short rain (SR) season runs from October to December of every year which annually averages between 430 mm and 350 mm for SR and LR season, respectively. The mean annual temperature is 21.6 °C where the climate is classified as tropical savanna based on Köppen climate classification. The soils are predominantly sandy loam, less weathered with good permeability, yellowish red, low pH and low soil organic carbon, Xanthic Ferrasols (Ngetich et al., 2014). The study area is characterised by relatively short seasons which are predominant in the drier low agricultural potential areas (Ngetich et al., 2014). However, the study has been found suitable for the low-land drought tolerant crop varieties of green grams, sorghum, cowpea, chicken pea, maize, common beans amongst other crops (Macharia et al., 2020).

# 2.2. Experimental design

The trial was established as researcher-managed, in a randomized complete block design (RCBD) with treatments replicated thrice. The experiment is composed of twelve different treatments containing organics, inorganics and their combinations alongside treatments with no external input of nutrients (control) under maize production. However, only four treatments were selected for this study on soil greenhouse gas quantification and simulation: i) inorganic fertiliser; ii) animal manure; iii) animal manure combined with inorganic fertiliser, the three applied at 120 kg N  $ha^{-1}$  yr<sup>-1</sup>; and iv) a control (no external inputs) (Macharia et al., 2020). Selection of the four treatments were based on their high adoption level in the area (Macharia et al., 2014). We sourced animal manure from the surrounding local farmers and which was later incorporated manually using hand hoes, a fortnight before planning. To supply the required 60 kg N  $ha^{-1}$  yr<sup>-1</sup> based on (FURP, 1987), we took a composite of three manure samples to the laboratory for analysis. Based on the manure results we applied 6 t  $ha^{-1}$  yr<sup>-1</sup> of dry goat manure for sole manure treatment and 3 t  $ha^{-1}$  yr<sup>-1</sup> for manure + fertiliser treatment. Mineral fertilisers were applied following the local practice during planting at the onset of the rains on 6<sup>th</sup> of April 2017 and 23<sup>rd</sup> of October 2017 for the two seasons under study. Manual land preparations were carried out by removing all the aboveground biomass at the beginning of each cropping season. The trial plots measured 6 m by 4.5 m with one meter as a buffer between plots and at least two meters between blocks and which were maintained weeds-free through hand hoeing, ensuring least soil disturbance. Dry highlands (DH 04) maize variety was planted as the test crop at 0.90 m inter-row by 0.60 m intra-row spacing.

# 2.3. The DNDC model

The Denitrification-Decomposition (DNDC) model version 9.5 was used in this study. The DNDC is a dynamic model of nitrogen (N) and carbon (C) biogeochemistry in agricultural ecosystems. The DNDC model framework includes edaphic, environmental, crop growth, C and N dynamics and trace gas emissions which are reported daily (Jarecki et al., 2018). The model was initially developed for quantifying C sequestration and emissions of greenhouse gas (Li et al., 1992). The first component contains sub-models for soil (texture, SOC, bulk density and soil hydraulic parameters), climate (solar radiation, wind speed, air temperature, humidity and precipitation), crop growth (water demand, crop type, C/N ratio, potential yield, optimal temperature and biomass fractions), agricultural management (irrigation, residue, fertiliser, harvest dates, tillage, and planting dates) and decomposition (microbial biomass, labile humus, litter and passive humus). The model converts primary drivers (human activity, climate, soil, and vegetation) into soil environmental factors (humidity, redox potential, pH, soil temperature and concentration gradients of substrates) (Zhang et al., 2018a; 2018b). The second component comprises of sub-models for denitrification, fermentation and nitrification and estimates both emissions and sequestration of N2O and CH<sub>4</sub> (Li, 2007).

#### 2.3.1. Model set up

Daily climatic data (rainfall (cm), maximum and minimum air temperature (°C), wind speed (m s<sup>-1</sup>), solar radiation MJ m<sup>-2</sup> d<sup>-1</sup> and relative humidity (%)) were collected using HOBO U30 NRC station data logger from an installed weather station within the experimental study site. The weather files for the above climate parameters for the period of study were prepared following DNDC guide (version 9.5). Soils were sampled from each of the plots prior to setting up of the experiment (February 2017) and taken to the laboratory for analysis following standard procedures as described by Macharia et al. (2020). They were tested for mineral nitrogen, bulk density, texture, soil organic carbon (SOC) and soil pH. Field capacity, slope, porosity, conductivity and wilting point had earlier on been determined in the same study site by Ngetich et al. (2014). Cropping data (the type of crop, planting and harvesting), tillage data (method of ploughing, day and month of land preparation, biomass fraction and biomass C/N ratio), fertiliser data (type, amount and method of fertiliser applied and the day and month of application) and manure amendments (type, amount, method of application and day and month applied) were all collected from the experiment as described in Macharia et al. (2020).

### 2.3.2. Model calibration and validation

The DNDC model was calibrated using measured field data from experimental plots. Grain yields were converted to carbon equivalent following the DNDC model user guide where 1 kg of Maize was taken to contain 0.4 kg of Carbon. It's worth noting that during calibration of the model, all crop and soil data were based on sample analysis in the laboratory from a field experiment outlined in section 2.2 and 2.3.

Model calibration portrayed a good fit between the field observations and model-simulated data with  $R^2$  ranging from 0.93–0.99 (Figure 1 a-p), and which were statistically similar at P = 0.05. This is an indication that the model was successfully calibrated and that the simulated data can be relied on for other purposes (García et al., 2014). From the measured and simulated data, the DNDC model tended to start the simulations slightly later than the measured values and with higher values compared to measured values (Figure 1). It was also observed that the simulated biomass increased in the last stage of plant growth - grain filling (Figure 1 d, h, i, p).

#### 2.4. GHG concentration determination and other field measurements

Vented manual static plastic chambers and gas chromatography were used to measure the two greenhouse gases: carbon dioxide -  $CO_2$ , and nitrous oxide -  $N_2O$  for a whole year (7<sup>th</sup> February 2017 to 6<sup>th</sup> February 2018).

The gas chambers comprised of a base and a lid, and which were inserted into the soils to a depth of 7 cm two weeks prior to our first sampling (Macharia et al., 2020). The chamber bases remained *in-situ* for the whole of the study period and only removed twice during key

agronomic activities such as manure incorporation and which coincided with land preparation. During sampling, the chamber bases and lids were held tightly together using metallic clips and deployed for a duration of 30 minutes. Gas sampling was generally on a weekly basis but also followed key agronomic activities such as weeding, rainfall events, manure and fertiliser application (Parkin and Venterea 2010). Sampling was done through gas pooling from three chambers per plot, measuring 6 m by 4.5 m, using 60 mL propylene syringe fitted with luerlocks. The chambers were deployed for 30 min (0, 10, 20 and 30 min). Gas samples were transferred to 20 mL pre-evacuated glass vials and taken to the laboratory for analysis at Mazingira Centre (ILRI--Nairobi, Kenya).

The gas chromatography (GC) comprised of  $^{63}$ Ni-electron capture detector (ECD) for determining the levels of concentration of N<sub>2</sub>O and a flame ionisation detector (FID) for determining the level of CO<sub>2</sub> in every vial. We utilized Nitrogen gas (N<sub>2</sub>) at 20 mL min<sup>-1</sup> flow rate as the carrier gas for both (ECD & FID) channels. To obtain the concentrations of each gas, a comparison between peak areas from the GC and peak areas of four calibration gas concentrations. We used linear regression determine the concentrations of CO<sub>2</sub> from the FID channel and a power function for the determination of N<sub>2</sub>O concentrations since the ECD channel assumes a non-linear dimension and power function results to better fits (Pavelka et al., 2018).

Biomass and grain yields were measured during same period as gas sampling and which were collected through destructive sampling done every two weeks from the  $21^{st}$  day after planting until harvest. Other measurements collected included soil water contents and soil temperature using Procheck at 0–10 cm depth. Meteorological data were collected using different sensors and archived in a HOBO U30 NRC station data logger. The GHG and biomass data were linearly interpolated between sampling dates for the whole year.



**Figure 1.** Comparison between the field-measured and DNDC simulated maize plant biomass for i) leaves (a, e, i, m), ii) stems (b, f, j, n), iii) roots (c, g, k, o), and iv) grain yields (d, h, i, p) from control, fertiliser, manure and manure + fertiliser plots, respectively, used for DNDC model calibration in Embu County, Kenya.

'able 1. Statistical evaluation of DNDC data	ily simulated (soil temperature and m	pisture) values in comparison with the measured	values in Embu County, Kenya.
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Treatment <sup>1</sup>	Measured	Simulated	Ν	E*	RMSE*	nRMSE (%)	ME	$\mathbb{R}^2$
Control	32.3	30.3	47	-2.05	14.20	44	0.93	0.19
Inorganic fertiliser	32.6	31.9	47	-0.70	4.86	15	0.98	0.27
Animal manure	32.9	31.5	47	-1.36	9.21	28	0.96	0.35
Manure + Fertiliser	32.6	31.9	47	-0.70	8.70	27	0.98	0.14
Control	0.11	0.11	47	0.01	0.04	9	0.93	0.40
Inorganic fertiliser	0.11	0.12	47	0.01	0.02	7	0.89	0.74
Animal manure	0.14	0.16	47	0.05	0.06	5	0.94	0.72
Manure + Fertiliser	0.12	0.14	47	0.05	0.05	5	0.92	0.32
	Treatment <sup>1</sup> Control Inorganic fertiliser Animal manure Manure + Fertiliser Control Inorganic fertiliser Animal manure Manure + Fertiliser	Treatment1MeasuredControl32.3Inorganic fertiliser32.6Animal manure32.9Manure + Fertiliser0.11Inorganic fertiliser0.11Animal manure0.14Manure + Fertiliser0.12	Treatment <sup>1</sup> Measured         Simulated           Control         32.3         30.3           Inorganic fertiliser         32.6         31.9           Animal manure         32.9         31.5           Manure + Fertiliser         32.6         31.9           Control         0.11         0.11           Inorganic fertiliser         0.11         0.12           Animal manure         0.14         0.16	Treatment <sup>1</sup> Measured         Simulated         N           Control         32.3         30.3         47           Inorganic fertiliser         32.6         31.9         47           Animal manure         32.9         31.5         47           Manure + Fertiliser         32.6         31.9         47           Control         0.11         0.11         47           Inorganic fertiliser         0.11         0.12         47           Animal manure         0.14         0.16         47           Manure + Fertiliser         0.12         0.14         47	Treatment <sup>1</sup> Measured         Simulated         N         E*           Control         32.3         30.3         47         -2.05           Inorganic fertiliser         32.6         31.9         47         -0.70           Animal manure         32.9         31.5         47         -0.36           Manure + Fertiliser         32.6         31.9         47         -0.70           Control         0.11         0.11         47         0.01           Inorganic fertiliser         0.11         0.12         47         0.01           Animal manure         0.14         0.16         47         0.05           Manure + Fertiliser         0.12         0.14         47         0.05	Treatment <sup>1</sup> Measured         Simulated         N         E*         RMSE*           Control         32.3         30.3         47         -2.05         14.20           Inorganic fertiliser         32.6         31.9         47         -0.70         4.86           Animal manure         32.9         31.5         47         -1.36         9.21           Manure + Fertiliser         32.6         31.9         47         -0.70         8.70           Control         0.11         0.11         47         0.01         0.04           Inorganic fertiliser         0.11         0.12         47         0.01         0.02           Animal manure         0.14         0.16         47         0.05         0.06           Animal manure         0.12         0.14         47         0.05         0.05	Treatment <sup>1</sup> Measured         Simulated         N         E*         RMSE*         nRMSE (%)           Control         32.3         30.3         47         -2.05         14.20         44           Inorganic fertiliser         32.6         31.9         47         -0.70         4.86         15           Animal manure         32.9         31.5         47         -1.36         9.21         28           Manure + Fertiliser         32.6         31.9         47         -0.70         8.70         27           Control         0.11         0.11         47         0.01         0.04         9           Inorganic fertiliser         0.11         0.12         47         0.01         0.02         7           Animal manure         0.14         0.16         47         0.01         0.02         5           Animal manure         0.14         0.16         47         0.05         0.06         5	Treatment1MeasuredSimulatedN $E^{\circ}$ RMSE $^{\circ}$ nRMSE (%)MEControl32.330.347-2.0514.20440.93Iorganic fertiliser32.631.947-0.704.86150.98Animal manure32.931.547-1.369.21280.96Manure + Fertiliser32.631.947-0.708.70270.98Control0.110.11470.010.0490.93Inorganic fertiliser0.140.16470.050.0650.94Animal manure0.120.44470.050.0550.92

\* The unit for E and RMSE is °C for soil temperature and m<sup>3</sup>m<sup>3</sup> for soil moisture.

<sup>1</sup> Treatments: Control = no external input, Inorganic fertiliser, Animal manure and Manure + fertiliser; the three applied at 120 kg N ha<sup>-1</sup> yr<sup>-1</sup>.

# 2.5. Model accuracy determination

To ascertain the general performance of the DNDC model, five statistical metrics were used to evaluate biomass production, maize yields, and daily soil moisture, temperature,  $N_2O$  and  $CO_2$  emissions between the measured and simulated values. They include mean error (ME), root mean squared error (RMSE), relative root mean squared error (rRMSE), model efficiency (ME) and the coefficient of determination ( $R^2$ ). Since using one of the metrics is not sufficient, a combination of the metrics gives a better response on the performance of the model as noted by Li et al. (2017).

# 2.6. Yield-scaled N<sub>2</sub>O emissions and N<sub>2</sub>O emission factors

We calculated yield-scaled nitrous oxide, which is a scale expressed as a unit (g) of  $N_2O$  emitted during production of a unit of grains (kg), by dividing cumulative annual  $N_2O$  emissions by annual grain yields. We also determined  $N_2O$  emission factors as shown in Eq. (1).

$$EF = \frac{(N_2 O - N_{fertilized}) - (N_2 O_{unfertilized})}{N_{applied}}$$
(1)

Where: " $N_2O$ - $N_{fertilised}$ " = annual N<sub>2</sub>O emissions from fertilised treatment, " $N_2O$ - $N_{unfertilised}$ " = annual N<sub>2</sub>O emissions from no external input treatment, and " $N_{applied}$ " = annual N rate

# 3. Results and discussion

#### 3.1. Soil temperature

The DNDC model accurately estimated daily soil temperature across treatments and which were a function of daily air temperatures. The simulated trends were in good agreement with the observed soil temperature, although slightly lower than the measured values indicating an underestimation of soil temperature by the model. Underestimation of soil temperature was highest from control plots (6%) and lowest in both inorganic fertiliser and manure combined with inorganic fertiliser treatments at 2% (Table 1). The simulated E ranged from -2.05 to -0.70 °C, RMSE from 4.86–14.20, nRMSE from 15–44%, ME from 0.93–0.98 while R<sup>2</sup> ranged from 0.14 to 0.35 across treatments (Table 1). The DNDC model performance was comparable with the one of Uzoma et al. (2015), who reported underestimation of soil temperature by DNDC in most of the years and whose estimate ranged between 5–8% between systems. The results also agree with Smith et al. (2008), who reported an average

Table 2. Comparison between the measured and the DNDC simulated crop growth under maize crop in in Embu County, Kenya.

Treatment <sup>1</sup>	Component	Measured (kg $ha^{-1}$ )	Simulated (kg ha <sup>-1</sup> )	E (kg ha <sup>-1</sup> )	RMSE	nRMSE (%)	ME
Control	Leaf	1570	1450	-120	85	5	0.92
	Stem	690	515	-175	124	18	0.75
	Roots	270	225	-45	32	12	0.83
	Grains	90	80	-10	7	8	0.89
	Total biomass	2620	2270	-350	247	43	0.87
Fertiliser	Leaf	2100	1990	-110	78	4	0.95
	Stem	1370	1290	-80	57	4	0.94
	Roots	460	357.5	-103	72	16	0.78
	Grains	310	215	-95	67	22	0.69
	Total biomass	4240	3853	-388	274	45	0.91
Manure	Leaf	3250	2975	-275	194	6	0.92
	Stem	1860	1613	-247	175	9	0.87
	Roots	610	580	-30	21	3	0.95
	Grains	2410	2190	-220	156	6	0.91
	Total biomass	8130	7358	-772	546	25	0.91
Manure + Fertiliser	Leaf	2200	1425	-775	548	25	0.65
	Stem	1230	847	-383	271	22	0.69
	Roots	430	238	-192	136	32	0.55
	Grains	220	190	-30	21	10	0.86
	Total biomass	4080	2700	-1380	976	88	0.66

<sup>1</sup> Treatments: Control = no external input, Inorganic fertiliser, Animal manure and Manure + fertiliser; the three applied at 120 kg N ha<sup>-1</sup> yr<sup>-1</sup>.

Table 3. Comparison between d	ily measured and	l simulated soil CO <sub>2</sub> and N <sub>2</sub>	O emissions from ma	aize crop in Embu	County, Kenya
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GHG	Treatment <sup>1</sup>	Measured	Simulated	N	Е	RMSE	nRMSE	ME	$R^2$
$CO_2$ (kg $CO_2$ -C ha <sup>-1</sup> d <sup>-1</sup> )	Control	$3.8^{\rm d}\pm0.20$	4.0	47	0.2	1.2	31	0.94	0.40
	Inorganic fertiliser	$5.2^{c}\pm0.30$	5.7	47	0.5	2.7	52	0.91	0.22
	Animal manure	$\textbf{9.8}^{a}\pm\textbf{0.31}$	10.6	47	0.8	4.1	42	0.93	0.62
	Manure + Fertiliser	$\textbf{7.4}^{b}\pm\textbf{0.45}$	7.5	47	0.2	2.9	39	0.98	0.60
	P value	< 0.001							
N <sub>2</sub> O (g N <sub>2</sub> O-N ha <sup>-1</sup> d <sup>-1</sup> )	Control	$0.36^d \pm 0.22$	0.4	47	-0.08	0.1	21	0.77	0.21
	Inorganic fertiliser	$1.07^{c}\pm0.36$	0.98	47	-0.08	0.4	40	0.92	0.39
	Animal manure	$3.34^{a}\pm0.33$	2.85	47	-0.49	2.6	77	0.85	0.24
	Manure + Fertiliser	$1.72^b\pm0.66$	1.64	47	-0.08	0.4	25	0.95	0.48
	P value	< 0.001							

The letters a,b,c & d in the Table denote significance of the statistical difference between treatment means (column difference).

<sup>1</sup> Treatments: Control = no external input, Inorganic fertiliser, Animal manure and Manure + fertiliser; the three applied at 120 kg N ha<sup>-1</sup> yr<sup>-1</sup>.

underestimation of 7% of soil temperature by DNDC model, across treatments. However, the results disagree with Li et al. (2017), who reported an overestimation of soil temperature in the range between 2–6% across cropping systems. It is worth noting that temperature influences soil moisture, microbial activities and evaporation. This implies that the accurate estimation by DNDC model is paramount since all these have a direct influence on GHG emissions and could have a direct effect towards accurate targeting of adaptation and mitigation measures. The relatively lower underestimation of soil temperature in plots treated with inorganic fertiliser, either sole or combined, could be ascribed to the model taking into consideration that inorganic fertilisers provides readily available nutrients for plant uptakes, promotes relatively faster crop growth, thus improving the canopy growth resulting to reduced thermal radiation along the soil profiles.

#### 3.2. Soil moisture

The DNDC model simulated daily trends of soil moisture content across treatments and which were primarily a function of precipitation. The model accurately simulated rainfall seasonality in the study site with moisture increasing to attain highest peaks at the onset of rainfall in each season. The DNDC model slightly overestimated moisture contents across treatments with the calculated E ranging from 0.01–0.05 m<sup>3</sup>m<sup>3</sup>, RMSE from 0.02-0.06 m<sup>3</sup>m<sup>3</sup>, nRMSE from 5-9%, ME from 0.89-0.94 and R<sup>2</sup> ranging from 0.32-0.74 (Table 1). Generally, the DNDC model overestimated soil moisture contents across treatments ranging between 9-17% with the highest overestimations recorded from plots treated with animal manure either sole or combined with inorganic fertiliser (Table 1). These results agree with Li et al. (2017), who recorded an overestimation of soil moisture content by DNDC model ranging between 2-8% across cropping systems. With the study period having recorded approximately 15% lower precipitation than seasonal average, these results were in agreement with Uzoma et al. (2015) who recorded an overestimated soil water content ranging from 15-21% in a relatively drier year. Results also agree with Smith et al. (2019) who recorded an overestimation of soil water content by DNDC model near soil surface and which was presumably caused by lack of root distribution algorithms, inability to simulate a heterogeneous soil profile and no water table. Further, results corroborate those of He et al. (2019) who reported an overestimation of soil water content by DNDC at 0-0.1 m depth and which was attributed to low root distribution algorithms in DNDC, and its inability to simulate heterogeneous soils. The overestimation could also be ascribed to the DNDC characterizing water flow in its hydrological sub-model between field capacity and wilting point (strictly) resulting to over-prediction of SWC (Dutta et al., 2016). The overestimation of soil moisture could result to high GHG emissions estimations which could result to inaccurate targeting of adaptation and mitigation measures. Results, however, disagree with Smith et al. (2008) who reported an

underestimation of soil moisture by the DNDC model by approximately 17%. It should be noted that continued application of manure in the study area resulted to increased soil organic matter (Macharia et al., 2020), and which could have ensured higher retention of water in plots treated with manure than plots without manure, a possible assumption made by DNDC model.

#### 3.3. Simulation of maize growth

The DNDC simulated seasonal crop production separated into different maize crop components (leaves, stems, roots and grain yields) were lower than the measured values across treatments (Table 2). This indicates that the DNDC model tended to underestimate crop production in the study area. Overall, plots treated with animal manure had highest amounts of carbon allocated along maize crop components, while control plots had least amounts of carbon allocated along maize plant components (Table 2). Underestimations were in the range of 5-35%, 6-31%, 5-45%, 9-31% and 9-34% for leaves, stems, roots, grains and total biomass, respectively, across treatments. Calculated E ranged from 350–1380 kg ha<sup>-1</sup>, RMSE from 247–976 kg ha<sup>-1</sup>, nRMSE from 25–88% and ME from 0.66-0.91 for total maize biomass across treatments (Table 2). The DNDC simulated data underestimated aboveground biomass (AGB) by 37% compared to the findings by Ngetich et al. (2014) in the same study site and who recorded an average AGB of 11.51 Mg  $ha^{-1}$  (4.60 Mg C  $ha^{-1}$ ) after application of inorganic fertiliser at 120 kg N  $ha^{-1} yr^{-1}$ .

The underestimation of maize crop productivity by the DNDC model could be ascribed to uneven rainfall distribution across the cropping year with most (64%) of rainfall during long rains season (LR 2017) being received during April while 96% of rainfall in the short rains season (SR, 2017) season being received in first month at the onset of rains rendering the rest of crop growing period to remain relatively dry as observed by Macharia et al. (2020). Results from this study agree with Zhang et al. (2018a; 2018b) who in their study reported that crop yields in years that reported low rainfall (similar to our study) were very likely to be underestimated in DNDC simulations. However, our results disagree with Muhammed et al. (2018) who reported a slight overestimation of crop production by the DNDC model.

# 3.4. Simulation of soil respiration

Daily simulated  $CO_2$  emissions ranged from 3.8–9.8 kg  $CO_2$ -C ha<sup>-1</sup> d<sup>-1</sup> and were slightly higher than measured emissions, which ranged from 4.0–10.6 kg  $CO_2$ -C ha<sup>-1</sup> d<sup>-1</sup> across treatments (Table 3). Overestimations of  $CO_2$  emissions ranged between 3–10% across treatments with manure + fertiliser recording lowest overestimations while inorganic fertiliser recorded highest overestimations. The simulated  $CO_2$  emissions were in good agreement with the measured emissions with a



Figure 2. Comparison between measured and simulated  $CO_2$  emissions from four different treatments; (a) control, (b) inorganic fertiliser, (c) animal manure, (d) animal manure + inorganic fertiliser in Embu County, Kenya and (e) Precipitation. The solid arrows show the timing of land preparation and manure incorporation, and the dotted arrows indicate the timing of planting and fertiliser application.

calculated E ranging from 0.2–0.8 kg CO<sub>2</sub>-C ha<sup>-1</sup> d<sup>-1</sup>, RMSE = 1.2–4.1 kg CO<sub>2</sub>-C ha<sup>-1</sup> d<sup>-1</sup>, nRMSE = 31–52%, ME = 0.91–0.94 and R<sup>2</sup> from 0.22–0.62 across treatments (Table 3). These daily emissions resulted in higher annual cumulative simulated CO<sub>2</sub> emissions that ranged from 1474–3860 kg CO<sub>2</sub>-C ha<sup>-1</sup> yr<sup>-1</sup> relative to measured CO<sub>2</sub> emissions which ranged from 1391–3574 kg CO<sub>2</sub>-C ha<sup>-1</sup> yr<sup>-1</sup> across treatments.

The DNDC simulated CO<sub>2</sub> emissions followed seasonality rising immediately after soil rewetting and which coincides with fertilization at the onset of the rains (Figure 2) similar to what was reported by Macharia et al. (2020). The CO<sub>2</sub> emission peaks were well-timed and accurately coincided with the measured peaks across treatments. These simulated CO<sub>2</sub> emission peaks could have been influenced by climate, fertilization regime and crop growth stage. The highest soil respiration peak during SR 2017 was 4.3 kg CO<sub>2</sub>-C ha<sup>-1</sup> day<sup>-1</sup> from manure treatment (Figure 2 c). It should be noted that during dry period, CO<sub>2</sub> emissions remained relatively low due to low microbial activities but upon soil rewetting, there was a pulse of CO<sub>2</sub> at onset immediately after a rainfall event (Figure 2). Similarly, immediately upon application of manure, there were no pulses of CO<sub>2</sub> emissions which could be because manure had not

decomposed due to its dryness, but upon addition of moisture from rainfall at onset, manure mineralised giving rise to  $CO_2$  peaks. The low  $CO_2$  emissions during this period could also be as a result of having no crop growing, therefore limited root respiration.

The low prediction of  $CO_2$  from control treatment could be attributed to low amounts of substrates for microorganism thus leading to low  $CO_2$ emissions while high amounts of  $CO_2$  emissions from animal manure treatment could be associated with easily available substrates from decomposition of organic materials. Overestimation in simulated data could be attributed to ability of DNDC model to factor in more dynamics of C fluxes occurring at the interface between terrestrial ecosystems and atmosphere compared with measured  $CO_2$  emissions. According to Li et al. (2010), simulated  $CO_2$  emissions include photosynthesis, plant autotrophic respiration, soil microbial heterotrophic respiration, and dissolved organic carbon (DOC) leaching. The slight overestimated soil moisture across the study period by the model which could have resulted to relatively higher microbial activities and enhanced plant root growth as measured by Uzoma et al. (2015). More so, higher  $CO_2$  emissions could have originated from the model underestimating crop growth hence allocating more carbon to be lost as  $CO_2$  emissions other than being sequestered by maize crop during its growth.

# 3.5. Simulation of soil $N_2O$ fluxes

The DNDC simulated N<sub>2</sub>O emissions rose immediately after soil rewetting and which coincided with fertilization and onset of rainy season (Figure 3). In most parts of the study period, the simulated  $N_2O$ emissions remained relatively lower than measured and which in the overall resulted in an underestimation of annual N2O emissions (Figure 3). Underestimations of N<sub>2</sub>O emissions ranged from 5-23% across treatments with manure combined with fertilisers recording the lowest while control recorded the highest underestimations, respectively. These results agree with Uzoma et al. (2015) and Yue et al. (2019) who found DNDC model to underestimate N2O emissions generally. Underestimation of N2O fluxes from current study could be attributed to semiarid soils in the study area remaining dry most of the year and therefore very little or no denitrification. Sandy loam soils, similar to soils in our study area, tend to dry up very fast after a rainfall event and probably the DNDC model was unable to accurately capture the abrupt changes in the soil water content, which doesn't last long before drying up. According to Smith et al. (2008), the DNDC model underestimations of N<sub>2</sub>O fluxes may be as a result of soil draining too quickly following rainfall, un-simulated lateral flow, or inaccurate model calculation of porosity. Further, Uzoma et al. (2015) noted that soil hydrology sub-model in DNDC model, have a cascade flow routine which drains the profile to field capacity, which likely underestimated denitrification events during a period of high rainfall shortly after fertiliser application at the onset, resulting to underestimation of  $N_2O$  fluxes.

All the daily simulations described temporal dynamics in N<sub>2</sub>O fluxes and which were generally in agreement with the measured N<sub>2</sub>O fluxes with an E ranging from -0.08 to -0.49, RMSE = 0.1–2.6, nRMSE = 21–77% while R<sup>2</sup> ranged from 0.21 to 0.48 (Table 3). The daily simulated data resulted to an annual cumulative N<sub>2</sub>O flux ranging from 100–1040 g N<sub>2</sub>O-N ha<sup>-1</sup> d<sup>-1</sup> compared to annual cumulative N<sub>2</sub>O fluxes ranging from 130–1220 g N<sub>2</sub>O-N ha<sup>-1</sup> d<sup>-1</sup> across treatments with control plots recording the least amounts while animal manure recorded the highest amounts of N<sub>2</sub>O fluxes, respectively.

In control plots, the low amounts of simulated N<sub>2</sub>O fluxes could be ascribed to low amounts of substrates while high amounts of N<sub>2</sub>O fluxes could be attributed to the availability of more labile C in the manure treatments providing the necessary condition for denitrification (Macharia et al., 2020). According to Li et al. (2010), manure amendment increases soil organic carbon which acts as a source of substrates for N<sub>2</sub>O stimulation through both soil nitrification and denitrification. It's worth noting that manure improves soil organic carbon build-up over time and which is capable of retaining soil moisture during the dry periods of cropping season, resulting in overall more denitrification.

The DNDC-simulated daily  $N_2O$  in peak emissions form, mainly come from both nitrification and denitrification processes. For this study, the simulated peaks for  $N_2O$  flux were well aligned with the timing of measured peaks which followed rainfall events with a slight difference in magnitude of simulated  $N_2O$  peaks (Figure 3). Our results are consistent



Figure 3. Measured and predicted  $N_2O$  fluxes from four different treatments; (a) control, (b) inorganic fertiliser, (c) animal manure and (d) animal manure + inorganic fertiliser in Embu County, Kenya. Solid arrows indicate timing of land preparation coinciding with incorporation of animal manure, while dotted arrows show timing of planting and fertiliser application.

Table 4. Comparison between measured and simulated yield-scaled N<sub>2</sub>O emissions and N<sub>2</sub>O emission factors (EF) from four different fertiliser treatments under maize crop in Embu County, Kenya.

Measured YSE <sup>2</sup>	Simulated YSE	Measured EF <sup>3</sup>	Simulated EF
$0.8^{c}\pm0.02$	0.9		
$1.1^{\rm b}\pm0.06$	1.1	0.2	0.2
$0.5^{c}\pm0.10$	0.5	0.9	0.8
$2.2^{a}\pm0.54$	2.5	0.4	0.4
	$\begin{array}{l} \mbox{Measured YSE}^2 \\ \mbox{0.8}^c \pm 0.02 \\ \mbox{1.1}^b \pm 0.06 \\ \mbox{0.5}^c \pm 0.10 \\ \mbox{2.2}^a \pm 0.54 \end{array}$	Measured YSE <sup>2</sup> Simulated YSE $0.8^c \pm 0.02$ $0.9$ $1.1^b \pm 0.06$ $1.1$ $0.5^c \pm 0.10$ $0.5$ $2.2^a \pm 0.54$ $2.5$	Measured YSE <sup>2</sup> Simulated YSE         Measured EF <sup>3</sup> $0.8^c \pm 0.02$ $0.9$ $1.1^b \pm 0.06$ $1.1$ $0.2$ $0.5^c \pm 0.10$ $0.5$ $0.9$ $0.9$ $2.2^a \pm 0.54$ $2.5$ $0.4$

The letters a,b,c & d in the Table denote significance of the statistical difference between treatment means (column difference).

<sup>1</sup> Treatments: Control = no external input, Inorganic fertiliser, Animal manure and Manure + fertiliser; the three applied at 120 kg N ha<sup>-1</sup> yr<sup>-1</sup>.

 $^2$  YSE = cumulative annual N<sub>2</sub>O emissions divided by the total grain yields (kg ha<sup>-1</sup> yr<sup>-1</sup>).

<sup>3</sup> Emission factors (EF) =  $N_2O$  difference between fertilized and unfertilized divided by annual N application rate.

with the findings of other studies which identified the DNDC model to generally capture the peaks of daily  $N_2O$  flux induced by precipitation, although slight discrepancies remained between magnitude of the modelled  $N_2O$  peaks and the corresponding observations (Uzoma et al., 2015; Deng et al., 2018). Simulated data also predicted more frequent  $N_2O$  peaks after rainfall events than field observations (e.g. mid-October to end of Dec 2017). This is consistent with Deng et al. (2018) who reported more frequent  $N_2O$  peaks after rainfall events during the rainy season than the measured peaks, which could not have been observed in field studies. As was observed by other  $N_2O$  modelling studies, accurate simulation of timing and daily  $N_2O$  flux variability possess a significant challenge (Smith et al., 2008; Uzoma et al., 2015).

#### 3.6. Yield-scaled N<sub>2</sub>O emissions and N<sub>2</sub>O emission factors (EF)

The DNDC simulated YSE were lowest from animal manure and highest from manure + fertiliser treatments (Table 4). Simulated YSE was similar for sole inorganic fertiliser and sole manure application but slightly higher than the observed for control (13%) and manure + fertilisers (14%) treatments. The relatively higher simulated YSE from control treatment could be attributed to highest (23%) N<sub>2</sub>O underestimation across treatments while that of manure + fertiliser could be more explained by underestimation (11%) of maize yields. It should be noted that YSE can evaluate trade-offs between crop production and environmental impacts under different soil fertility management technologies (Van Groenigen et al., 2010). The YSE from this study were relatively lower compared with what has been observed within the region and which ranged between 0.7 and 41.6 g  $N_2O$ -Nkg<sup>-1</sup> N aboveground biomass. These YSE could be attributed to low N<sub>2</sub>O emissions rather than to high crop yields due to the inherent soil fertility challenges experienced in the study area (Macharia et al., 2020). The simulated N2O emission factors (EF) were lowest (0.2%) from inorganic fertiliser and highest (0.8%) in animal manure treatment (Table 4). Simulated N<sub>2</sub>O EFs were similar to observed values for sole inorganic fertiliser and manure + fertiliser but slightly (14%) lower than observed value for animal manure treatment (Table 4).

## 4. Conclusion

The results indicate that the DNDC-simulated soil temperature and soil moisture contents were lower than and higher than the measured values from experimental site, respectively, suggesting that the DNDC model tended to underestimate soil temperature by 2–6% and overestimate SWC by 9–17% across treatments. Further, the DNDC model tended to underestimate crop growth by 2–45% for all the maize crop component (*i.e.* leaves, stems, roots and grains). Still, it accurately simulated treatment performance across treatments with animal manure and control, producing the highest and the lowest total biomass, respectively. The DNDC simulated soil respiration (CO<sub>2</sub>) was in good agreement with the measured values though they were slightly higher by 3–10% compared to measured values from the experimental site, attributed to the relatively higher simulated SWC resulting in enhanced soil and root respiration. The DNDC-simulated CO<sub>2</sub> emissions followed seasonality, remaining relatively low during dry periods and having high peaks upon rewetting and fertilization at the onset of the rains. For N<sub>2</sub>O emissions, the DNDC simulated values were slightly lower than the measured values (5-23%) a factor attributed to the fact that the model is unable to capture abrupt changes in the soil water content from sandy soils which tends to dry up almost immediately after a rainfall event, thus provoking lower denitrification. Similar to CO<sub>2</sub> simulated values, the DNDC model followed seasonality for N2O emissions but had more peaks than measured values. The simulated data captured well the timing of the N<sub>2</sub>O fluxes with a slight variation in the magnitude of the N2O fluxes. Further, the simulated N2O YSE was similar with the measured values for sole manure and sole fertiliser but slightly higher for control (12%) and manure combined with inorganic fertiliser (14%) while the EFs were similar for sole inorganic fertiliser and manure combined with inorganic fertiliser but slightly lower for sole manure treatment (11%). With all the EFs from this study ranging between 1.25 to 5 folds lower than the IPCC Tier I emission factors (1%), and which were overall in good agreement with the measured values, we conclude that DNDC model is an accurate and reliable model which can be used to simulate emission factors which could be used as a credible alternative by the developing nations to report to the United Nations Framework Convention on Climate Change (UNFCCC) on their agriculture-based NDCs in line with Paris Agreement of 2015. Further, the DNDC model could be used to fill the huge data gaps in developing countries on GHG emissions, attributed to the paucity of observation data on GHG emissions due to the high cost involved in direct GHG quantification studies resulting to uncertainty in national GHG inventories. More so, DNDC model could also be applied across different regions across countries in confidently simulating EF from different soil management practices thus bringing out the nexus between improved agricultural productivity and reduced GHG emissions across different agricultural soil types and landscapes. However, attention should be paid to the fluxes due to the slight underestimation of  $\mathrm{N_2O}$  and slight overestimation of CO2 fluxes. We, therefore, recommend the establishment of more similar studies across sub-Saharan African which could act as a source of data for the continued model improvement hence target to achieve correct climate change adaptation and mitigation measures across the region.

# Declarations

# Author contribution statement

Joseph M. Macharia: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Felix K. Ngetich: Conceived and designed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Chris A. Shisanya: Contributed reagents, materials, analysis tools or data; Wrote the paper.

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#### Data availability statement

Data will be made available on request.

#### Declaration of interests statement

The authors declare no conflict of interest.

# Additional information

No additional information is available for this paper.

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