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In-situ N_2O and N_2 data improved N budget simulation with APSIM and LandscapeDNDC in tropical sugarcane systems

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ABSTRACT

Denitrification is a key process in the global nitrogen (N) cycle, causing nitrous oxide (N_2O) and dinitrogen (N_2) emissions. Biogeochemical models allow field-scale estimates of N_2O and N_2, extrapolating important yet often limited experimental results. However, such predictions rely mostly on N_2O data, and the lack of N_2 data hinders validating total denitrification, which remain a major uncertainty for N budgets. This study investigated denitrification losses and N budgets in two tropical sugarcane systems using the Agricultural Production Systems sIMulator (APSIM) and the LandscapeDNDC (LDNDC) simulation framework using a unique dataset of both N_2O and N_2 emissions measured in the field over a complete growing season. Key soil N parameters influencing N_2O and N_2 emissions in APSIM and LDNDC were identified via global sensitivity analysis, followed by generalised likelihood uncertainty estimation to determine their posterior distributions using (i) N_2O data only and (ii) both N_2O and N_2 data. The simulation of N_2O emissions in APSIM and LDNDC were improved in both calibration approaches, resulting in 0.7–1.3 kg N ha^{-1} of RMSE. However, simulated N_2 emissions increased and agreed better with the observed values only when calibrated with both N_2O and N_2 (RMSE 30.1–45.0 kg N ha^{-1} before calibration and 19.3–19.9 kg N ha^{-1} after). The simulated N loss pathway shifted from leaching to N_2 emissions after calibration including N_2. The simulated N balance was larger when sugarcane residues were retained as compared to burning consistently across the different soil N parameter configurations. These findings indicate that biogeochemical models, when used with default soil N parameters or calibration limited to N_2O data, are likely to underestimate denitrification losses (>50 %), leading to a bias in N budgets simulation. Accurate N loss estimates are essential for understanding the long-term management impacts on soil organic matter dynamics, as demonstrated by the improved N budgets from both simulation models denote N mining when sugarcane is burnt, and the potential to sequester N when cane residues are retained. These outcomes emphasise the importance of integrating in-situ measurements of N_2O and N_2 in simulation exercises, ensuring more accurate N budget estimates across scales.

1. Introduction

Agriculture is responsible for approximately two-thirds of all environmental harmful (N) losses to the environment (Sutton et al., 2013), pushing the global N flow beyond planetary boundaries (Richardson et al., 2023). The accumulation of reactive N (N_r) in the biosphere is causing a range of severe environmental issues, including eutrophication, biodiversity loss, human health problems and perturbations of the climate system (Erisman et al., 2013). Losses of N to the environment are mainly caused by excessive N inputs, surpassing the crop N demand at the farm level (McLellan et al., 2018). Strategies of N fertiliser management thus need to account for N losses to minimise environmental impacts while maintaining crop productivity and farm profitability (Mueller et al., 2014).

Denitrification is a key soil N transformation process and N loss pathway, reducing nitrate (NO_3^-) to gaseous N emissions mainly in the

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form of nitrous oxide (N_2O) and dinitrogen (N_2). Emissions of N_2O contribute to climate change, as N_2O is a long-lived atmospheric trace gas with a global warming potential 273 times higher than that of carbon dioxide (CO_2) over a 100-year period (IPCC, 2021) and the greatest remaining threat to the stratospheric ozone layer (Portmann et al., 2012; Ravishankara et al., 2009). Emissions of N_2 are environmentally benign, but a loss of N from the system (Takeda et al., 2023) and a direct economic loss with potentially further detrimental effects on crop growth and therefore agricultural productivity. Despite a growing body of denitrification research delivering both N_2O and N_2 data, measuring N_2 emissions from the soil against the high atmospheric N_2 background remains challenging (Friedl et al., 2020; Groffman et al., 2006), reflected in the small number of studies quantifying both N_2O and N_2 in the field. Due to the lack of in situ N_2O and N_2 data, denitrification as a critical determinant of N_r losses remains a major uncertainty in the N budget of agroecosystems.

Mechanistic biogeochemical models offer a powerful tool for estimating N budgets at the field scale, complementing field experiments where it is impractical to measure comprehensive N budgets. Models, like the Agricultural Production System sIMulator (APSIM) (Holzworth et al., 2014; Thorburn et al., 2010) and LandscapeDNDC (LDNDC) (Haas et al., 2013), can simulate N cycling within the plant-soil-atmosphere continuum. These models simulate denitrification losses as functions and interactions of water content, temperature, pH, carbon (C) availability and NO_3^- content in the soil (Del Grosso et al., 2020; Farquharson and Baldock, 2008; Heinen, 2006), allowing estimation of emissions under diverse environmental and management conditions.

However, the mechanistic understanding of denitrification in these models is currently based on a limited number of incubation results (Del Grosso et al., 2000; Parton et al., 1996), and the capacity of biogeochemical models to simulate N cycling has been largely evaluated by plant N uptake, mineral N dynamics and N_2O emissions, serving as a proxy for denitrification rates (De Antoni Migliorati et al., 2021; Gurung et al., 2021; Mielenz et al., 2017, 2016; Necpálová et al., 2015). Other major N losses, such as leaching, are often not measured, resulting in poorly constrained N loss pathways and thus N budget estimates. The lack of comprehensive field data on complete denitrification losses leads to an inconsistency in N cycling across models (Fuchs et al., 2020). The need for further validation with field measurements including N_2 emissions has been highlighted (Del Grosso et al., 2020; Grosz et al., 2023; Reading et al., 2019; Thorburn et al., 2011) to reduce uncertainty in N budget estimation.

To address this issue, this study employed both APSIM and LDNDC together with a unique calibration dataset of both N_2O and N_2 in intensively managed sugarcane (*Saccharum* spp.) systems (Takeda et al., 2023). The study applied a combination of global sensitivity analysis, Bayesian calibration and uncertainty analysis to assess the capacity of these models to simulate N budgets depending on N_2O and N_2 data availability. We hypothesise that using N_2 data would increase the magnitude of denitrification while shifting its product ratio towards N_2 in the model, given the dominance of N_2 shown in the field study, which would further alter the relative importance of N loss pathways in simulation. Accurate N budgets will improve our understanding of the impacts of farming practices on reactive and non-reactive N losses from soil and the model intercomparison based on unique in-situ data can highlight potential areas for model improvement.

2. Materials and methods

We tested the Agricultural Production Systems sIMulator (APSIM) (Holzworth et al., 2014) and the biogeochemical model framework LandscapeDNDC (LDNDC) (Haas et al., 2013) for simulation of N cycling in tropical sugarcane systems in Australia with the observed data including plant N uptake, N_2O emissions and N_2 emissions (Takeda et al., 2023).

2.1. Study site and experimental design

The field experiments were conducted on commercial sugarcane farms in Burdekin, QLD (19° 37' 4'' S, 147° 20' 4'' E) from October 2018 to August 2019 and in Mackay, QLD (21° 14' 4'' S, 149° 04' 6'' E) from October 2019 to August 2020, and described in detail in Takeda et al. (2022). The climate in both Burdekin and Mackay is tropical. The soil is classified as Brown Dermosol and Brown Kandosol in the Australian Soil Classification (Isbell, 2016), or Luvisol and Fluvisol in the World Reference Base (WRB) Classification (IUSS Working Group.. 2014), at the Burdekin and Mackay sites, respectively. Sugarcane varieties Q240 and Q208 were planted in 2015 and 2016 and the crop was the third ratoon during the experiment at the Burdekin and Mackay sites, respectively. Irrigation was applied by furrow irrigation at the Burdekin site and overhead sprinkler at the Mackay site. Sugarcane is burnt before harvest to remove the leaves at the Burdekin site, leaving little trash (crop residues) on the ground. 'Green cane trash blanketing (GCTB)', a practice where the cane is harvested green and the trash is spread over the ground, is practised at the Mackay site. Selected soil and management properties are shown in Table 1.

A detailed description of the experimental design and setup at the Burdekin and Mackay sites can be found in Takeda et al. (2021a) and Takeda et al. (2022), respectively. Fertiliser N rate treatments applied as urea N included an unfertilised control (0 N), 150 kg N ha^{-1} (150 N), 200 kg N ha^{-1} (200 N) and 250 kg N ha^{-1} (250 N), plus 100 kg N ha^{-1} (100 N) at the Mackay site only. The recommended N rate based on the district yield potential and soil C content (i.e. the SIX EASY STEPS program of the Australian sugar industry) (Schroeder et al., 2010) was 150 N at the Mackay site and 200 N at the Burdekin site. Urea was applied by banding the fertiliser 0.1 m deep and 0.3 m from the bed centre on both sides of the cane row at the Burdekin site and by stool splitting 0.1 m deep at the bed centre of the cane row at the Mackay site.

High temporal resolution measurements of N_2O emissions were conducted (Takeda et al., 2022, 2021a) using automated greenhouse gas monitoring systems (Grace et al., 2020). Together with in-situ ^{15}N gas flux method (Friedl et al., 2017), field-scale N_2 emissions were quantified over the crop-growing season (Takeda et al., 2023). Sugarcane yield, biomass and N uptake were measured at harvest. Auxiliary measurements included soil temperature, water content, ammonium (NH_4^+) content and NO_3^- content (Takeda et al., 2023).

2.2. Crop models – APSIM

The Agricultural Production Systems sIMulator (APSIM, version 7.10) (Holzworth et al., 2014) was used for the simulation analyses,

Table 1
Soil properties at 0–0.2 m depth and crop management practices at the Burdekin and Mackay sites.

		Burdekin	Mackay
Soil (0.0–0.2 m)	BD (g cm^{-3})	1.3	1.1
	pH (H_2O)	6.92	4.13
	Total C (%)	1.60	1.35
	Total N (%)	0.08	0.09
	Clay (%)	35.4	22.2
	Silt (%)	26.0	15.9
	Sand (%)	38.7	61.9
Crop management	Cultivar	Q240	Q208
	Crop	3rd ratoon	3rd ratoon
	N rate treatments (kg N ha^{-1})	0, 150, 200 and 250	0, 100, 150, 200 and 250
	N fertiliser product	Urea	Urea
	Fertiliser application	Two-sided banding	Stool splitting
	Irrigation management	Furrow	Overhead
	Trash management	Burnt	GCTB

which is one-dimensional with a daily-time step. APSIM has the capacity to represent important features of sugarcane production systems including residue decomposition (Thorburn et al., 2001); nitrification (Meier et al., 2006a); denitrification (Thorburn et al., 2010); NO_3^- in runoff (Vilas et al., 2022) and deep drainage (Stewart et al., 2006). The APSIM model was configured with modules for soil N and C (APSIM-SoilN) (Probert et al., 1998), soil water (APSIM-SoilWat) (Probert et al., 1998), sugarcane growth (APSIM-Sugarcane) (Keating et al., 1999) and crop residue decomposition (within APSIM-SurfaceOM) (Probert et al., 1998). The soil profile was configured down to 1.5 m with 0.1–0.3 m of depth increments. In APSIM-SoilN, nitrification-related parameters, the maximum reaction velocity (V_{max}) and NH_4^+ concentration at the half potential rate (K_m) were reduced from default values (V_{max} = 40 μg N g^{-1} soil day^{-1} and K_m of 90 mg N g^{-1} soil) to V_{max} = 12 μg N g^{-1} soil day^{-1} and K_m of 30 mg N g^{-1} (Meier et al., 2006b; Smith et al., 2020). In APSIM, the denitrification process is described as a first-order decay process accounting for NO_3^- and labile C contents as substrate availability and also soil moisture and temperature as limiting factors in each soil layer (Thorburn et al., 2010). The denitrified N is then partitioned into N_2O and N_2 emissions, not considering potential losses of nitric oxide (NO). APSIM-Sugarcane and APSIM-SurfaceOM were configured based on the recent study on Australian sugarcane systems (Biggs et al., 2021).

2.3. Crop models – LandscapeDNDC

LandscapeDNDC (LDNDC, version 1.35.2) is a framework for terrestrial ecosystems models of biogeochemical C and N cycling that has emerged from the generalization of the DNDC 9.3 (Smith et al., 2010) for arable systems and PnET-N-DNDC (Li et al., 2000) for forest systems (Haas et al., 2013). The models describe different processes in ecosystem domains, e.g. microclimate, water cycle, plant physiology and soil biogeochemistry. The chosen model setup included the vegetation model PlaMo^x (Kraus et al., 2016; Liebermann et al., 2020; Petersen et al., 2021), the biogeochemical model MeTr^x (Kraus et al., 2015) and the water cycle model WatercycleDNDC (Kiese et al., 2011) for simulations. Similar to APSIM, the chosen model setup considers the ecosystem one-dimensional with a soil profile down to 2.0 m with 0.05–1.0 m of depth increments. The temporal resolution was set to one hour. Sugarcane-specific parameters for PlaMo^x were set manually fitted based on observed cane yield and plant N uptake. The MeTr^x soil bio-geochemistry module simulates soil C and N turnover and the associated processes of humification, mineralisation, nitrification, denitrification and ammonia (NH_3) volatilisation (Kraus et al., 2014). Decomposition of organic matter originating from plant litter input or root exudates delivers NH_4^+ to the soil. Mineralised N may be further transformed by microbes to nitrite, NO_3^-, NO, N_2O or N_2 via the microbial processes of nitrification and denitrification, leached, immobilised by plants or the microbial community or lost along hydrological and gaseous pathways. Microbial N (and C) processing is simulated on the basis of Michaelis-Menten kinetics, thereby considering the effects of changes in soil environmental conditions on soil microbial processes, specifically soil moisture and temperature, but also pH or texture.

2.4. Climate and soil inputs across models

Climate inputs were generated from the historic weather data using Scientific Information for Land Owners (SILO) climate stations and interpolated gridded database (Jeffrey et al., 2001) and supplemented with on-site measurements where available. Base soil inputs were retrieved from the Soil and Landscape Grid of Australia (SLGA) database (Grundy et al., 2015) and estimated using pedotransfer functions (Palmer et al., 2017). Soil inputs were then updated with on-site measured data down to 1.0 m (the bottom layer data was extended for the deeper soil layers in the model) for soil texture, bulk density, organic carbon content and pH. Soil physical properties (soil water content at air dry, lower limit, field capacity and saturation, as well as saturated and unsaturated hydraulic conductivities) were adjusted to fit the observed soil water content dynamics. Model performance of soil temperature, water content, NH_4^+ content and NO_3^- content simulations is shown in Figs. S1–4.

2.5. Global sensitivity analysis- Extended-FAST

The key soil N parameters in APSIM and LDNDC which influence N_2O and N_2 emissions were identified via a global sensitivity analysis using the extended Fourier amplitude sensitivity test (extended-FAST) (Saltelli et al., 1999). The extended-FAST assesses the relative importance of parameters to the output of interest, reducing the number of parameters to calibrate (Sexton et al., 2017). In this analysis, the parameters relevant mainly to production and emissions of N_2O and N_2 from APSIM and LDNDC were considered (Table 2). From each parameter distribution, 1000 values were sampled, leading to 7000 parameter sets in APSIM and 12,000 in LDNDC to simulate both N_2O and N_2 emissions for each combination of site and N rate treatment. The contribution of each parameter alone ("main effect") and in combination with other parameters ("interaction effect") to the variance of simulated N_2O and N_2 emissions was calculated across the sampled parameter sets and reported by averaging across sites and N rates for each parameter. The sensitive parameters were determined by the threshold of the main sensitivity index > 5 % or the sum of main and interaction indices > 10 % on average for either N_2O or N_2 emissions.

2.6. Bayesian calibration – Generalised Likelihood Uncertainty Estimation (GLUE)

Generalised Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992), one of the most applied informal Bayesian calibration methods, was used to calibrate the models and simultaneously quantify the uncertainty in parameter values (Sexton et al., 2016). GLUE determines the posterior (i.e. calibrated) parameter distributions as a function of likelihood (i.e. the probability of observed data assuming a parameter set) and the prior parameter distributions (assumed uniform within the range in this study, Table 2). The parameters identified as influential on N_2O or N_2 emissions in the global sensitivity analysis (using extended-FAST) were involved in this calibration analysis and 50, 000 parameter sets were generated by Latin hypercube sampling from the prior parameter distributions. The likelihood function followed the probability density function of normal distribution (He et al., 2010; Sexton et al., 2016) and the likelihood calculated across N rates at each site was combined across output variables by the mathematical product (i.e. the sum of the log-likelihood) (He et al., 2010). The variables to fit with the observed data were (i) seasonal cumulative N_2O emissions only and (ii) both seasonal cumulative N_2O and N_2 emissions. The parameter sets resulting in the best 1 % of the combined likelihood (Vrugt et al., 2009) were selected and the posterior parameter distribution was approximated by kernel density estimation of the selected parameter values (Gurung et al., 2020).

2.7. Uncertainty analysis

Parameter-induced uncertainty was evaluated for N_2O and N_2 emissions as well as plant N uptake by Monte Carlo simulation with 500 parameter sets sampled from the posterior parameter distributions (Myrgiotis et al., 2018; Vrugt et al., 2009). The uncertainty range was determined as the 95 % credible intervals by calculating the 2.5 % and 97.5 % percentiles of the simulation outputs.

2.8. Statistical analysis

Statistical analyses and graphical presentations in this study were conducted using R statistical software version 4.0.3. (R Core Team,

Table 2
Default, lower limit, and upper limit values and assumed prior distribution of APSIM and LandscapeDNDC (LDNDC) parameters related to denitrification and N_2O emission algorithms, which are included in the global sensitivity analysis.

Model	Parameter	Description	Default	Lower limit	Upper limit	Prior distribution
APSIM	dnit_rate_coeff	Denitrification rate coefficient (kg soil mg^{-1} C d^{-1})	0.0006	0.0001	0.005	Uniform
	dnit_wf_power	Power term for calculation of water factor for denitrification	1	0.2	5	Uniform
	wfps_lim	Lower limit of WFPS to trigger denitrification	DUL	0.6	0.85	Uniform
	dnit_k1	A parameter for calculating N_2O fraction related to gas diffusivity in soil at field capacity	1.7 – 25.1	1	120	Uniform
	dnit_wfps	WFPS for calculating N_2O fraction of denitrification (lower limit)	21	10	50	Uniform
	dnit_n2o_factor	WFPS factor for N_2O fraction of denitrification (upper limit)	1.18	0.5	2.5	Uniform
	nit_n2o_frac	Fraction of nitrified nitrogen lost as N2O	0.002	0.0005	0.005	Uniform
LDNDC	d_eff_reduction	Reduction factor for gas diffusion.	1	0.1	10	Uniform
	mic_eff	Microbial carbon use efficiency	0.848	0.1	2	Uniform
	kmm_c_mic	Michaelis-Menten factor for carbon dependency of microbial growth	0.0010	0.0001	0.0100	Uniform
	kmm_n_mic	Michaelis-Menten factor for nitrogen dependency of microbial growth	0.0010	0.0001	0.0100	Uniform
	f_denit_m_weibull_1	Factor for water filled pore space dependency of denitrification	0.65	0.1	1	Uniform
	f_denit_m_weibull_2	Factor for water filled pore space dependency of denitrification	15	5	30	Uniform
	f_denit_n2_max	Factor determining the maximum fraction of denitrified nitrogen converted to N_2	0.85	0.7	1	Uniform
	f_denit_n2_min	Factor determining the minimum fraction of denitrified nitrogen converted to N_2	0.6	0.2	0.7	Uniform
	f_denit_no	Exponential factor determining how much denitrified nitrogen goes to NO.	8	1	10	Uniform
	kmm_c_denit	Michaelis-Menten factor for carbon dependency of denitrification	0.00200	0.00001	0.01000	Uniform
	kmm_n_denit	Michaelis-Menten factor for nitrogen dependency of denitrification	0.0020	0.0001	0.0100	Uniform
	muemax_c_denit	Growth rate of denitrifying microbes.	0.5	0.1	10	Uniform

2020) with a significant level set at $P < 0.05$. The R package *lhs* was used to sample parameter sets by the Latin hypercube method (Carnell, 2022). The R package *sensitivity* was used to implement extended-FAST (Iooss et al., 2022). The model simulation performance was evaluated by comparing simulated values with observed mean values per treatment using the coefficient of determination (R^2), the root mean square error (RMSE) and the normalised RMSE (nRMSE).

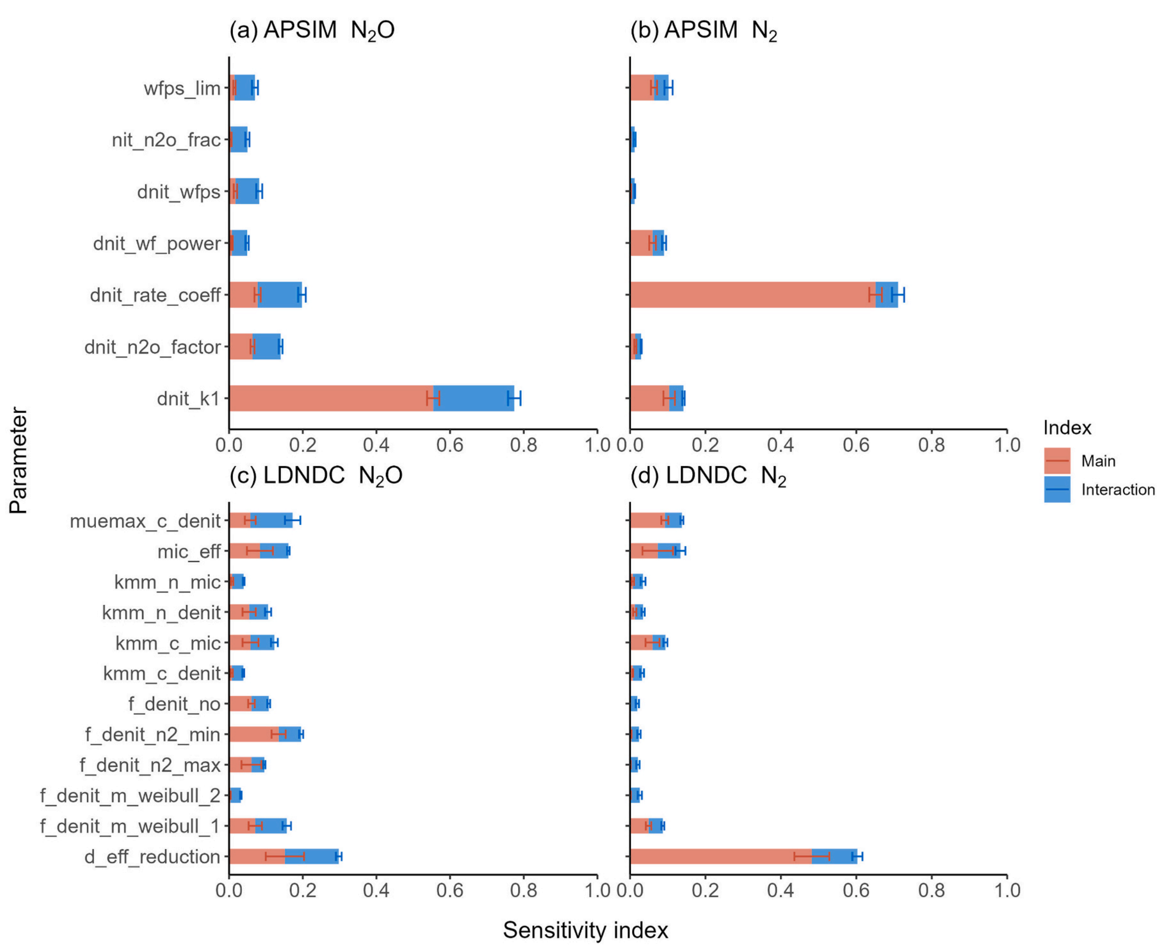

Fig. 1. Sensitivity indices showing contribution of each parameter alone ("main") and in combination with other parameters ("interaction") to the variance of simulated cumulative N_2O (a and c) and N_2 (b and d) emissions at harvest on average across two sites and N rate treatments in APSIM (a and b) and LandscapeDNDC (LDNDC) (c and d).

3. Results

3.1. Sensitive parameters and calibrated parameter distributions

The global sensitivity analysis with extended-FAST identified parameters that significantly influenced N_2O and N_2 emissions, narrowing down the number of parameters to be calibrated to five for APSIM and six for LDNDC (Fig. 1). The calibration analysis using GLUE (Fig. 2 and Table 3) resulted in the posterior parameter distributions differing between the two calibrations (both N_2O and N_2 or N_2O only) and/or between the sites.

3.1.1. In APSIM

The denitrification rate coefficient (*dnit_rate_coeff*), was identified as the most influential parameter for N_2 emissions, and the second most influential for N_2O emissions (Fig. 1). The parameter related to soil diffusion and its role in determining the ratio between N_2O and N_2 (*dnit_k1*) was the most influential on N_2O emissions and the second most influential on N_2 emissions. Parameters related to the effect of soil water on denitrification (*wfps_lim* and *dnit_wf_power*) were also identified as influential on N_2 emissions. The parameter controlling the ratio between N_2O and N_2 in response to soil moisture (*dnit_n2o_factor*) had a significant effect on N_2O emissions.

The most Influential parameter, *dnit_rate_coeff* was larger when calibrated with both N_2O and N_2 emissions (0.00199 on average across sites) compared to when calibrated with N_2O only (0.00111) (Fig. 2). The parameter value with the highest probability of the posterior distribution was close to the default value at the Burdekin site (0.00063) but greater at the Mackay site (0.00275) when calibrated with both N_2O and N_2. The parameters related to the ratio between N_2O and N_2 (*dnit_k1* and *dnit_n2o_factor*) largely increased from the default values (~25.1 and 1.18) at both sites when calibrated with both N_2O and N_2 (82.9 and 2.07 on average across sites, respectively). The parameters related to the WFPS dependency of denitrification (*wfps_lim* and *dnit_wf_power*) did not differ between the two calibrations but differed between the sites (0.69 and 4.2 at the Burdekin site and 0.62 and 0.79 at the Mackay site, respectively, when calibrated with N_2O and N_2).

3.1.2. In LDNDC

The reduction factor for gas diffusion (*d_eff_reduction*) was the most influential for both N_2O and N_2 emissions (Fig. 1). Both N_2O and N_2 emissions were also sensitive to parameters associated with the WFPS dependency of denitrification (*f_denit_m_weibull_1*), carbon dependency of microbial growth (*kmm_c_mic*), growth rate of denitrifying microbe (*muemax_c_denit*) and microbial carbon use efficiency (*mic_eff*). For N_2O emissions, the factor determining the minimum fraction of denitrified nitrogen converted to N_2 (*f_denit_n2_min*) was also influential.

The most influential parameter on both N_2O and N_2 emissions, *d_eff_reduction*, was close to the default value (1.0) across sites when calibrated with both N_2O and N_2 (1.35, Table 3) while much larger at the Mackay site when calibrated with N_2O only (6.9, Fig. 2). The minimum fraction of denitrified nitrogen converted to N_2 (*f_denit_n2_min*) were larger at the Burdekin site (0.55) compared to the Mackay site (0.47), where the parameter decreased to around 0.3 if only N_2O was used for calibration. The growth rate of denitrifying microbe (*muemax_c_denit*) increased largely from the default value (0.50) across sites, especially when calibrated with both N_2O and N_2 (5.43). Michaelis-Menten factor for carbon dependency of microbial growth (*kmm_c_mic*) also increased compared to the default value (0.0010) and was greater at the Mackay site (0.0057) than at the Burdekin site (0.0034). The parameter of WFPS dependency of denitrification (*f_denit_m_weibull_1*) was greater when calibrated with N_2O only (0.69) compared to when calibrated with both N_2O and N_2 (0.60) on average across sites.

3.2. Simulated N_2O and N_2 emissions over the sugarcane growing season

Simulated daily N_2O and N_2 emissions for the first four months after fertilisation with 200 kg N ha^{-1} are shown in Figs. 3 and 4, for the Burdekin and Mackay sites, respectively. Simulated daily N_2O and N_2 emissions at other N rates for the full crop growing season are shown in Figs. S6, S7, S8 and S9. Comparison between observed and simulated cumulative N_2O and N_2 emissions as well as plant N uptake at harvest is summarised in Fig. 5 across models, sites and treatments.

3.2.1. In APSIM

At the Burdekin site, APSIM overestimated peak N_2O emissions by > 400 g N ha^{-1} in the first three months after fertilisation when the default parameters were used (Fig. 3a), while N_2 emissions were simulated reasonably well (Fig. 3c). APSIM, when calibrated with N_2O data only, simulated N_2O emissions close to the observed emissions (Fig. 3a) but underestimated N_2 emissions (Fig. 3c) by 26.1–44.0 kg N ha^{-1} across the fertilised treatments (Figs. 5b and 5c). The calibration with both N_2O and N_2 data resulted in the first few N_2 emission peaks overestimated and the late N_2 peaks underestimated (Fig. 3c), but enabled APSIM to simulate both N_2O and N_2 emissions well at the cumulative scale ranging from 0.3 to 3.6 kg N ha^{-1} and from 2.9 to 76.4 kg N ha^{-1}, respectively (Figs. 5b and 5c). At the Mackay site, APSIM with default parameters underestimated N_2O and particularly N_2 emissions by up to 60 kg N ha^{-1} (Figs. 5b and 5c). Calibrating APSIM with either N_2O only or both N_2O and N_2 improved the simulation of both N_2O and N_2 emissions, smoothing the emissions between peaks (Figs. 4a and 4c) and resulting in 0.3–5.3 and 6.7–100.9 kg N ha^{-1} of cumulative N_2O and N_2 emissions, respectively (Figs. 5b and 5c). However, underestimation of the late N_2O and N_2 peaks at around three months after fertilisation remained in the low N fertiliser rate treatments even after calibration using both N_2O and N_2 data (Figs. S7a and S8a).

3.2.2. In LDNDC

At the Burdekin site, LDNDC achieved a reasonable match with the observed cumulative N_2O and N_2 values with the default parameters, ranging from 0.3 to 3.1 kg N ha^{-1} and from 3.7 to 84.3 kg N ha^{-1}, respectively (Figs. 5b and 5c). Calibrating LDNDC with either N_2O only or both N_2O and N_2 did not change the cumulative emission estimates (Figs. 5b and 5c), but the parameter-induced uncertainty decreased when both N_2O and N_2 were used for calibration compared to N_2O only (Figs. 3b and 3d).

At the Mackay site, LDNDC with default parameters underestimated N_2O emissions at the low N fertiliser rates and N_2 emissions across all N rates (Figs. 5b and 5c). Calibration with N_2O data alone improved N_2O by increasing the magnitude of peak N_2O emissions reaching 200 g N ha^{-1} and ranging from 0.1 to 4.6 kg N ha^{-1} at cumulative, but not N_2 emissions (Figs. 4b, 4d, 5b and 5c). Calibration with both N_2O and N_2 data significantly improved N_2 simulation resulting in 3.6–75.8 kg N ha^{-1} of cumulative emissions, but underestimation of both N_2O and N_2 emissions remained in the low N fertilization treatments, especially during late emission peaks (Figs. S7b and S8b).

Across sites and models, the model performance to simulate seasonal plant N uptake did not largely differ between calibrations with nRMSE values ranging from 21.2–23.1 % in APSIM and 15.4–19.3 % in LDNDC (Table 4). Between the models, APSIM simulated greater plant N uptake than LDNDC across the sites (Fig. 5a). The calibration with either N_2O only or both N_2O and N_2 reduced RMSE of N_2O considerably from 6.6 to 1.2–1.3 kg N ha^{-1} (> 250–44.6 %–48.0 % of nRMSE) in APSIM and 1.1–0.7–0.9 kg N ha^{-1} (43.2–26.6 %–35.5 % of nRMSE) in LDNDC (Table 4). The calibration with N_2O alone reduced RMSE of N_2 emissions only in APSIM from 43.7 to 30.1 kg N ha^{-1} while increasing RMSE of N_2 emissions from 39.6 to 45.0 kg N ha^{-1} in LDNDC (Table 4). The calibration with both N_2O and N_2 data improved both N_2O and N_2 estimates consistently in both models compared to the default configuration, resulting in the RMSE of N_2 emissions at 19.9 and 19.3 kg N ha^{-1}

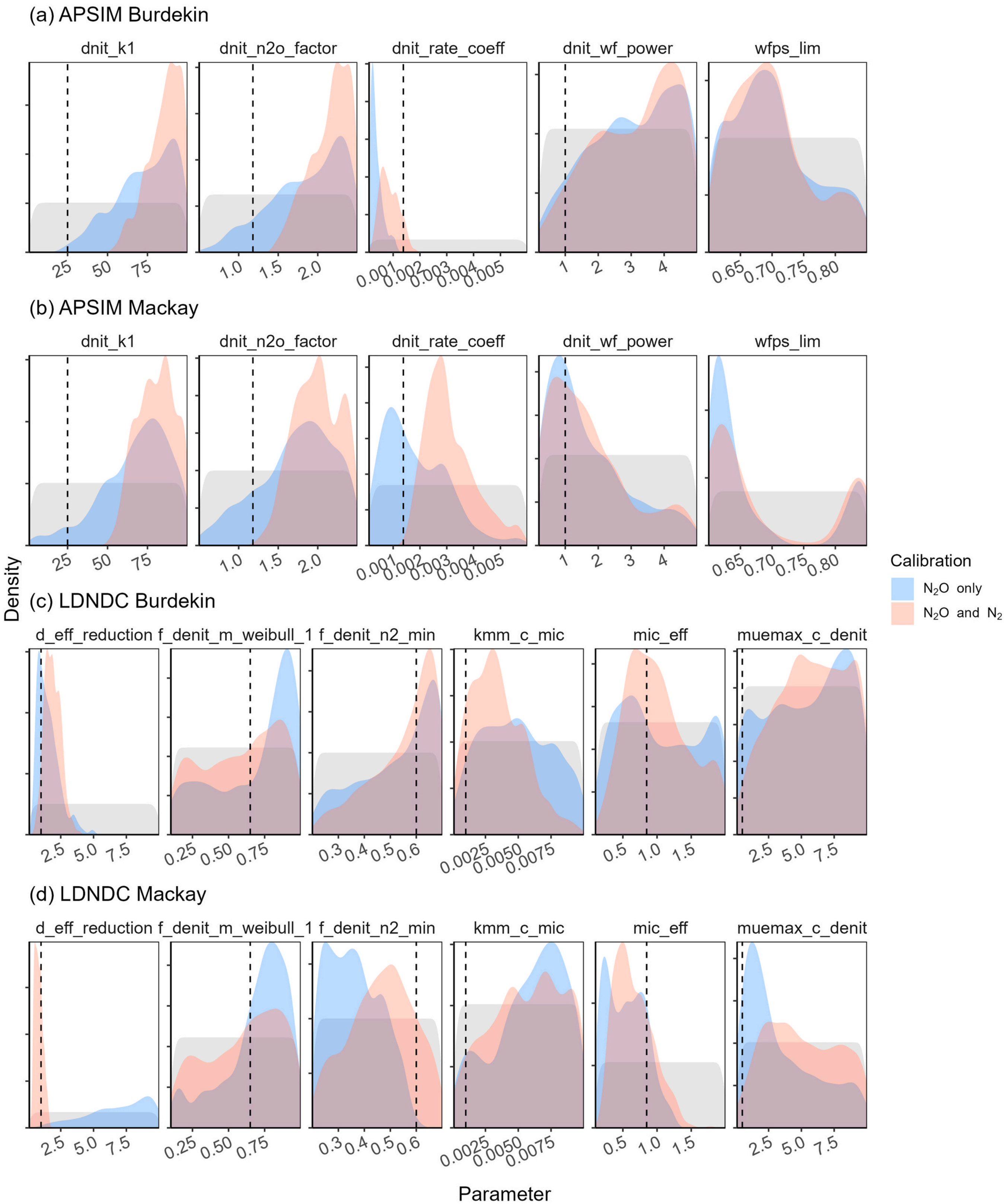

Fig. 2. Posterior distributions of APSIM (a and b) and LandscapeDNDC (LDNDC) (c and d) parameters calibrated using generalised likelihood uncertainty estimation (GLUE) with N_2O only (blue area) or N_2O and N_2 (red area) data at the Burdekin (a and c) and Mackay (b and d) sites. For each parameter, values with greater density means higher probability based on respective calibration. The vertical dashed line and grey shaded area indicate the default parameter value and the prior parameter distribution, respectively.

Table 3

Descriptive statistics (mean, median, maximum a posteriori (MAP), standard deviation (SD), lower limit (LL) and upper limit (UL) of 95 % credible intervals (CI)) of mixture posterior distribution of the APSIM and LandscapeDNDC (LDNDC) parameters calibrated with both N_2O and N_2 across the Burdekin and Mackay sites.

Model	Parameter	Default	Mean	Median	MAP	SD	95 % CI LL	95 % CI UL
APSIM	dnit_rate_coeff	0.00138	0.00199	0.00167	0.00077	0.00133	0.00035	0.00498
	dnit_wf_power	1	2.43	2.22	1.43	1.43	0.28	4.85
	wfps_lim	DUL	0.697	0.672	0.624	0.082	0.603	0.847
	dnit_k1	1.7–25.1	82.9	84.4	87.7	11.4	59.8	99.4
	dnit_n2o_factor	1.18	2.07	2.09	2.34	0.28	1.51	2.49
LDNDC	d_eff_reduction	1	1.35	1.21	0.76	0.72	0.41	2.91
	f_denit_m_weibull_1	0.65	0.598	0.638	0.845	0.259	0.134	0.980
	f_denit_n2_min	0.6	0.509	0.522	0.643	0.131	0.235	0.693
	kmm_c_mic	0.00100	0.00456	0.00421	0.00321	0.00265	0.00038	0.00967
	mic_eff	0.848	0.839	0.759	0.571	0.417	0.270	1.875
	muemax_c_denit	0.50	5.43	5.39	4.46	2.70	0.70	9.75

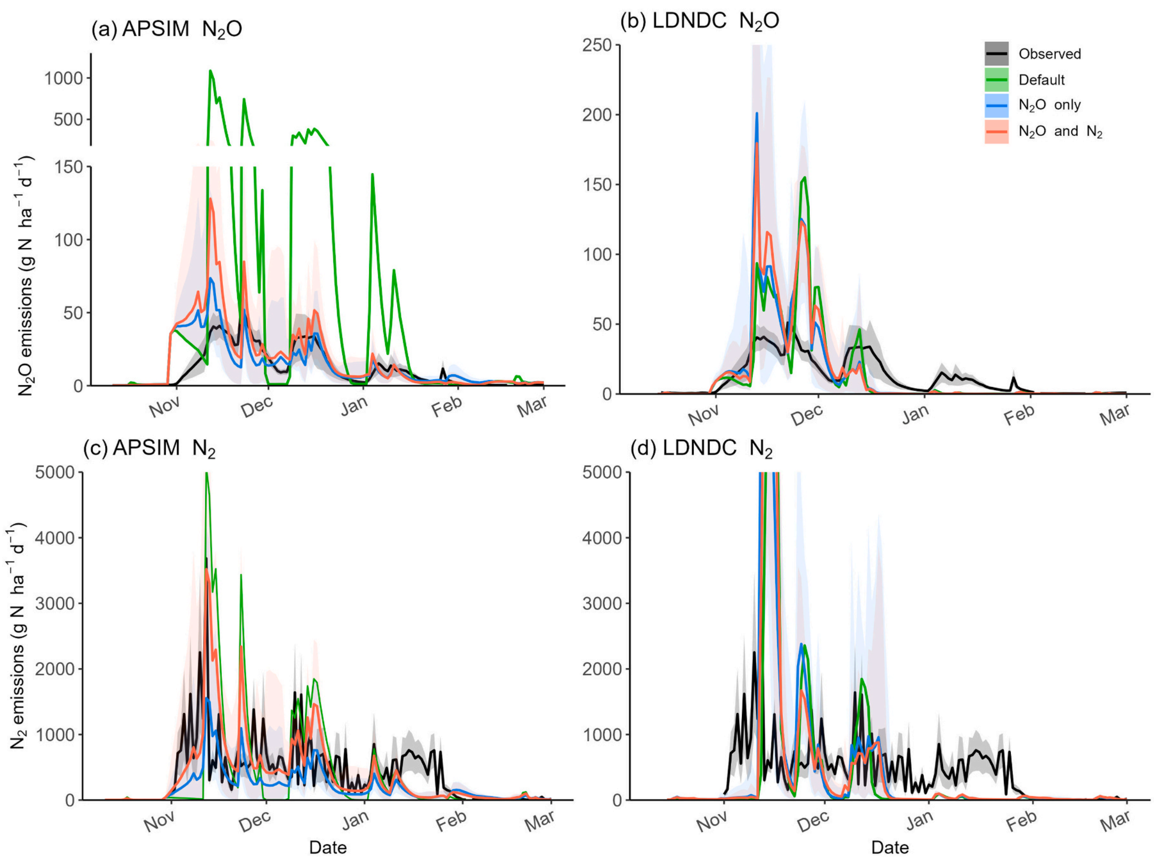

Fig. 3. Emissions of N_2O (top, a and b) and N_2 (bottom, c and d) observed (black) and simulated in APSIM (left, a and c) and LandscapeDNDC (LDNDC) (right, b and d) with the calibrated parameters with both N_2O and N_2 data (red), the calibrated parameters only with N_2O data (blue) and the default parameters (green) over four months after fertilisation at 200 kg N ha^{-1} of N fertiliser rate at the Burdekin site.

(34.3 % and 33.2 % of nRMSE) in APSIM and LDNDC, respectively (Table 4). On average across sites and N rates, the underestimation of denitrification losses (N_2O+N_2) with both models with default parameters (55 % and 53 % in APSIM and LDNDC, respectively) persisted after calibration with N_2O data only (50 % and 54 %) but improved when calibrated with both N_2O and N_2 data (24 % and 26 %).

3.3. Simulated N budgets

The major pathways of N exports from the sugarcane systems were N_2 emissions, leaching and plant N via harvest and burning in both APSIM and LDNDC irrespective of soil N parameter configuration, accounting for > 94 % of the sum of N exports (Fig. 6). In general, N exports increased with N application rates. At 0 N, N losses via denitrification and leaching were < 10 and < 5 kg N ha^{-1} respectively across sites, models and parameter configurations. For the highest N application rate, these values increased to > 80 and > 30 kg N ha^{-1}, largely varying across models and calibration strategies.

Among denitrification losses, N_2O emissions accounted for only a small portion (< 2 %) of the N budget, except for > 10 kg N ha^{-1} of N_2O emissions simulated at N rates > 150 kg N ha^{-1} by APSIM with the default parameters. When calibrated with either N_2O only or both N_2O and N_2, the simulated N_2O emissions using APSIM were up to 3.3 and 5.3 kg N ha^{-1} at 250 N at the Burdekin and Mackay sites, respectively. In LDNDC, the simulated N_2O emissions were up to 2.9 and 4.7 kg N ha^{-1} at the Burdekin and Mackay sites, respectively.

Emissions of N_2 simulated responded to both N rates and calibration strategies. In APSIM, the simulated N_2 emissions were 41 and 73 kg N ha^{-1} at 250 N at the Burdekin and Mackay sites, respectively, when calibrated with N_2O data only. When calibrated with both N_2O and N_2,

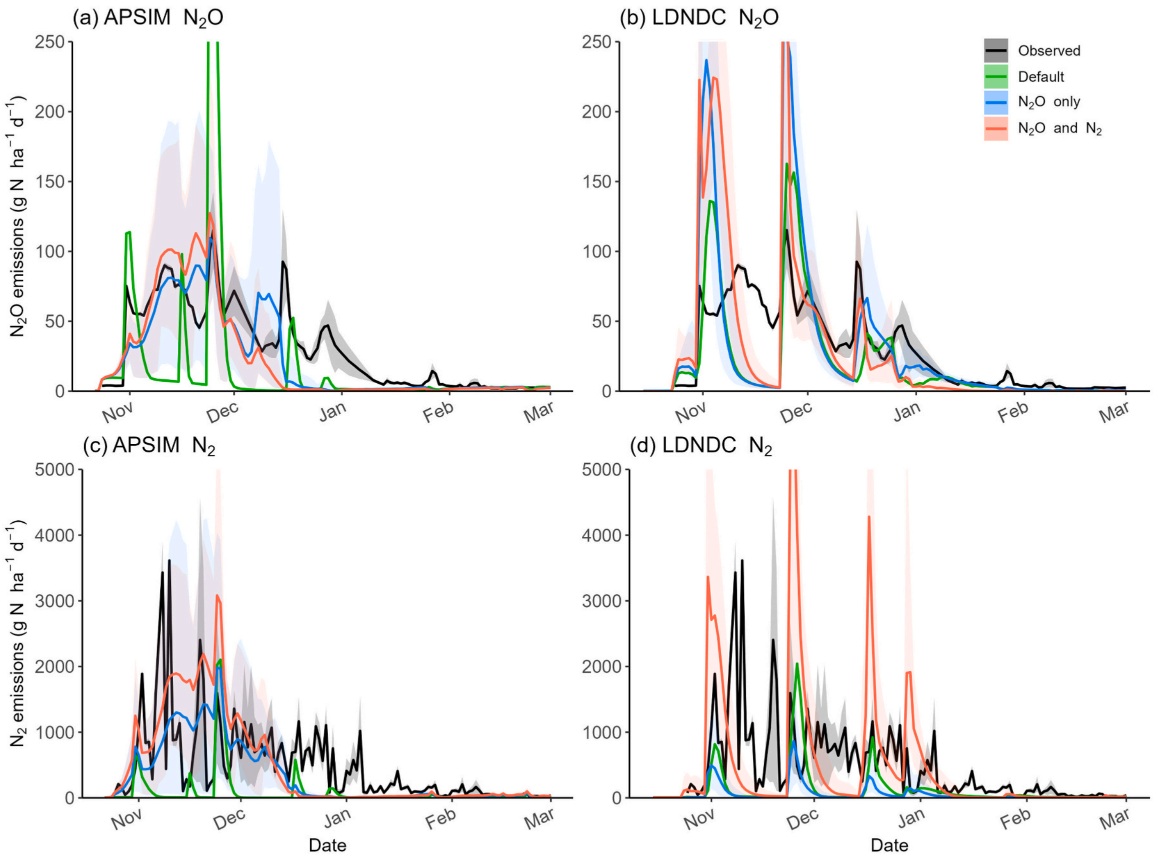

Fig. 4. Emissions of N_2O (top, a and b) and N_2 (bottom, c and d) observed (black) and simulated in APSIM (left, a and c) and LandscapeDNDC (LDNDC) (right, b and d) with the calibrated parameters with both N_2O and N_2 data (red), the calibrated parameters only with N_2O data (blue) and the default parameters (green) four months after fertilisation at 200 kg N ha^{-1} of N fertiliser rate at the Mackay site.

these values increased to 76 and 101 kg N ha^{-1}. In LDNDC, the corresponding values were 86 and 9 kg N ha^{-1} when calibrated with N_2O only, and 83 and 76 kg N ha^{-1} when calibrated with both N_2O and N_2. On average across models, sites and N rates, simulated N_2 emissions accounted for 19 % and 33 % of the N input when calibrated with N_2O only and both N_2O and N_2, respectively.

Loss of N via leaching varied between models and also in response to the calibration strategies. In APSIM, the simulated N leaching was 60 and 5 kg N ha^{-1} at 250 N at the Burdekin and Mackay sites when calibrated with N_2O only, which decreased to 30 and 1 kg N ha^{-1} when calibrated with both N_2O and N_2. In LDNDC, the loss of N via leaching was 4 and 139 kg N ha^{-1} at 250 N at the Burdekin and Mackay sites, when calibrated with N_2O only, and the calibration with both N_2O and N_2 decreased leaching N loss to 61 kg N ha^{-1} only at the Mackay site. On average across models, sites and N rates, simulated N loss via leaching accounted for 16 % and 5 % of the N input when calibrated with N_2O only and both N_2O and N_2, respectively.

For other minor N loss pathways, APSIM simulated $<$ 3 kg N ha^{-1} of N loss via runoff and LDNDC simulated $<$ 2 kg N ha^{-1} of NH_3 volatilisation as well as $<$ 4 kg N ha^{-1} of NO emissions, across the two sites and the different soil N parameter configurations.

In contrast, N exported via uptake are consistent between models and across the soil N parameter configurations, while differing between sites. In APSIM, N exported via uptake was 82–87 kg N ha^{-1} at 0 N and 168–179 kg N ha^{-1} at 250 N at the Burdekin site, and 27–33 kg N ha^{-1} at 0 N and 63–93 kg N ha^{-1} at 250 N at the Mackay site. In LDNDC, the simulated N uptake exported was 24–34 at 0 N and 142–150 at 250 N at the Burdekin site, and 21–30 kg N ha^{-1} at 0 N and 64–74 kg N ha^{-1} at 250 N at the Mackay site.

Overall, the N balance (i.e. N input via fertilisation minus the sum of N export include harvested and burnt plant N, leaching, runoff and gaseous N losses) was larger at the Mackay site compared to the Burdekin site consistently across the different soil N parameter configurations, moderately increasing with N rates and differing between the models (Fig. 6). At 0 N, the N balance was negative since no N fertiliser was applied, resulting in -62 and -36 kg N ha^{-1} at the Burdekin and Mackay sites, respectively, on average across the models and the different soil N parameter configurations. In APSIM, the N balance ranged from -43 to -32 kg N ha^{-1} at the Burdekin site, and from 26 to 93 kg N ha^{-1} at the Mackay site, on average across the different soil N parameter configurations. In LDNDC, the corresponding values were -3–13 kg N ha^{-1} at the Burdekin site, and 15–41 kg N ha^{-1} at the Mackay site.

4. Discussion

The capacity of biogeochemical models to simulate N cycling has been mostly evaluated by plant N uptake, mineral N dynamics and N_2O emissions as a proxy for denitrification. However, these evaluations have been constrained by limited data availability, typically focusing on single N rates and short measurement periods, thus leaving denitrification as a major uncertainty in these models (Del Grosso et al., 2020; Grosz et al., 2021; Thorburn et al., 2010). This study, for the first time, leverages field-measured N_2 and N_2O emissions across various N rates to assess the capabilities of APSIM and LDNDC in simulating denitrification and N budgets. The unique field dataset improved soil N parameter estimates, which greatly reinforced the reliability of denitrification and thus N budget simulation within APSIM and LDNDC, highlighting the potential consequences in environmental impact assessments as well as the space in denitrification algorithms to refine further.

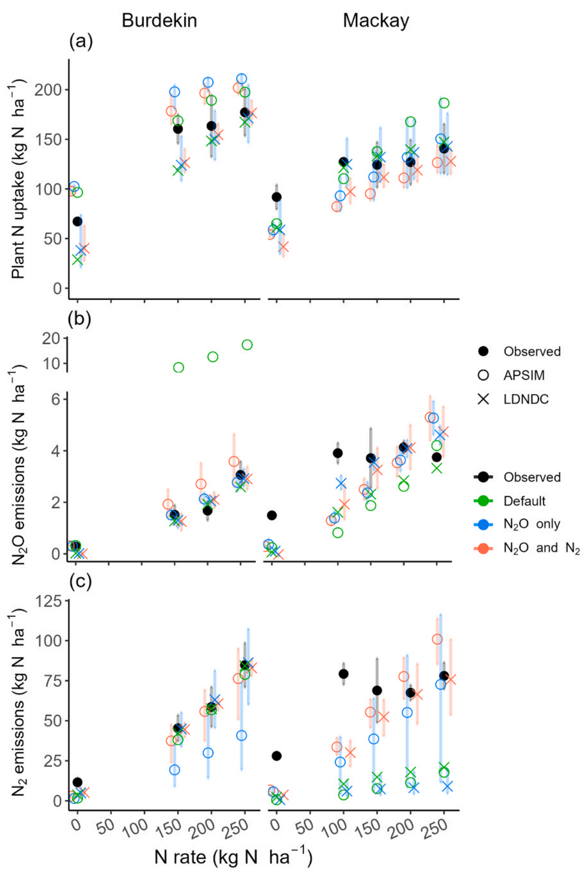

Fig. 5. Plant N uptake (a), seasonal N_2O emissions (b) and seasonal N_2 emissions (c) observed (filled circle) and simulated in APSIM (empty circle) and LandscapeDNDC (LDNDC, cross) with the calibrated parameters with both N_2O and N_2 data (red), the calibrated parameters only with N_2O data (blue) and the default parameters (green) across N rates from 0 to 250 kg N ha^{-1} at the Burdekin (left) and Mackay (right) sites.

Table 4
APSIM and LandscapeDNDC (LDNDC) simulation performances (R_2, RMSE and nRMSE) for plant N uptake, N_2O emissions, N_2 emissions and fertiliser N loss with default parameters, parameters calibrated with N_2O only and parameters calibrated with N_2O and N_2.

		APSIM			LDNDC		
Parameter	Variable	R^2	RMSE (kg N ha^{-1})	nRMSE (%)	R^2	RMSE (kg N ha^{-1})	nRMSE (%)
Default	Plant N uptake	0.74	27.8	21.2	0.80	23.2	17.7
	N_2O	0.00	6.6	250.7	0.67	1.1	43.2
	N_2	0.16	43.7	75.3	0.20	39.6	68.2
Posterior mean (N_2O only)	Plant N uptake	0.74	30.3	23.1	0.84	20.2	15.4
	N_2O	0.50	1.2	44.6	0.83	0.7	26.6
	N_2	0.60	30.1	51.9	0.10	45.0	77.6
Posterior mean (N_2O & N_2)	Plant N uptake	0.69	29.3	22.3	0.92	25.3	19.3
	N_2O	0.41	1.3	48.0	0.71	0.9	35.5
	N_2	0.66	19.9	34.3	0.67	19.3	33.2

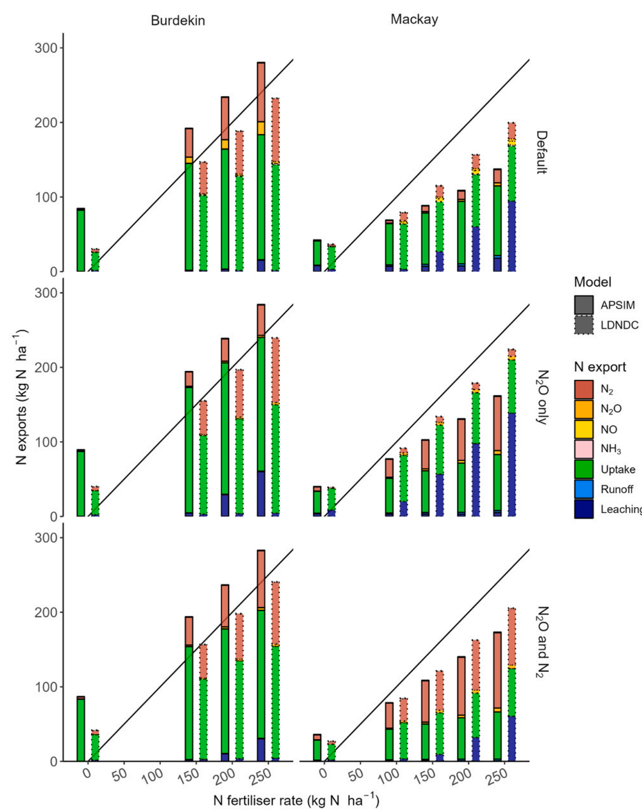

Fig. 6. N exports (sum of leaching, runoff, NH_3, NO, N_2O, N_2 and plant uptake) simulated in APSIM (solid line around) and LandscapeDNDC (LDNDC, dotted line around) with the parameters at default (top), calibrated only with N_2O data (middle) and calibrated with both N_2O and N_2 data (bottom) across N fertiliser rates from 0 to 250 kg N ha^{-1} at the Burdekin (left) and Mackay (right) sites. The black solid line shows 1:1 line, and the sum of N exports above and below this line indicate negative and positive N balance over the crop growing season, respectively.

4.1. *Importance of N_2 data to constrain N cycle simulation in biogeochemical models*

The key APSIM parameters identified in this study (Fig. 1) agree with those often calibrated to fit N_2O emissions such as *dnit_rate_coeff*, *dnit_wf_power* and *dnit_k1* in the previous modelling exercises (Bilotto et al., 2021; Li et al., 2021; Thorburn et al., 2010). Similarly, the key parameters in LDNDC (e.g. *d_eff_reduction*, *mic_eff* and *muemax_c_denit*, Fig. 1) were overlapped with those aiming at simulating N_2O emissions (Houska et al., 2017; Liebermann et al., 2020; Myrgiotis et al., 2018). As demonstrated in this study, N_2 emissions were sensitive to the parameters directly associated with the calculation of total denitrification losses while N_2O emissions were sensitive to those parameters and even more to the parameters relevant to the partitioning of denitrification products (Fig. 1). This indicates the model parameters identified influential on N_2O emissions can still serve as the candidate parameters to calibrate for denitrification simulation.

The calibration analyses showed considerable shifts in key soil N parameters from the default values and also difference between calibrations with N_2O only and both N_2O and N_2 (Fig. 2). Calibrating the models with N_2O data only, resulted in well-matched seasonal N_2O emissions relative to the observed values while N_2 emissions were consistently underestimated, with the exception of APSIM at the Burdekin site (Fig. 5). The disagreement in N_2 emissions highlights the limitations of using N_2O emissions as a sole proxy for denitrification losses, reflected in the calibrated parameters highly influential on N_2 emissions differing between the two calibrations such as *dnit_rate_coeff* in

APSIM and *d_eff_reduction* in LDNDC (Fig. 2). Combining both N_2O and N_2 data for calibration resulted in larger N_2 emissions (Fig. 5) and the ratio between N_2 and N_2O sifted towards N_2 except for LDNDC at the Burdekin site (Fig. S9), where both emissions were simulated well with the default parameters and thus the parameters did not change much by the calibrations. Emissions of N_2O accounted for 3 %–5 % of N_2O+N_2 in the previous field study (Takeda et al., 2023), and 11 % in a global meta-analysis (Scheer et al., 2020). The models calibrated with both N_2O and N_2 resulted in the corresponding value of 5 % in APSIM and 4 % in LDNDC agreeing well with the observed values, but the models with default parameters of calibrated with N_2O only lead to 13 % and 15 % on average, respectively. Our findings suggest that using default parameters or calibration with N_2O data alone not only underestimates the magnitude of denitrification but also the fraction emitted as N_2.

Prior attempts to calibrate the denitrification modules in the applied models have typically relied on N_2O measurements as a proxy for denitrification in the absence of N_2O+N_2 data in APSIM (Li et al., 2021; Mielenz et al., 2016) and LDNDC (Houska et al., 2017). Emissions of N_2O in these models are derived from the magnitude of total denitrification and the respective product ratios (e.g. N_2:N_2O), which are rarely validated due to the lack of field N_2 data. Either of these uncertainties in total denitrification and product ratios can therefore result in the same magnitude of N_2O emissions, but with significant differences in total denitrification loss. This study clearly demonstrated that calibration with N_2O data only can improve simulation of N_2O emissions but may compromise the simulation of N_2 emissions, leading to substantial errors in the complete N budget. This finding underscores the need for utilizing both N_2O and N_2 data to effectively constrain biogeochemical models, ensuring accurate and comprehensive simulations of denitrification losses.

4.2. Comparison between sites and models for further model improvement in denitrification algorithms

The calibration, using both N_2O and N_2 data, resulted in comparable model performance in simulating seasonal N_2O and N_2 emissions between APSIM and LDNDC (Table 4). However the posterior distribution of certain parameters in each model differed between sites (Fig. 2), which likely reflect the difference in the current denitrification algorithms. For example, APSIM simulates total denitrification as first-order kinetics with a constant denitrification rate coefficient (*dnit_rate_coeff*) in relation to substrate (NO_3^-) and labile organic carbon availability. Conversely, LDNDC simulates the denitrification rate as Michaelis-Menten kinetics and calculates microbial N demand that is converted from the carbon demand of denitrifiers based on a combination of their growth rate (*muemax_c_denit*) and carbon use efficiency (*mic_eff*). In this particular case, the Michaelis-Menten kinetics in LDNDC resulted in a more consistent calibration results between sites compared to the first-order kinetics in APSIM (Fig. 2), but there is by far no general consensus on the structure of denitrification algorithms in biogeochemical models (Heinen, 2006).

The calibrated models exhibited differences in simulating peaks and drops of N_2O and N_2 emissions (Figs. 3 and 4), which are likely associated with the model structure and parameters triggering denitrification in response to soil water dynamics. In the case of APSIM, denitrification is simulated when soil WFPS exceeds a certain threshold (*wfps_lim*) and gas products are assumed to be directly released to the atmosphere. This WFPS threshold parameter in APSIM differed between sites (Fig. 1), corroborating the variability of this threshold across soil types demonstrated in the previous modelling study (Mielenz et al., 2016). Instead of direct association with WFPS, LDNDC simulates denitrification activity based on the soil anaerobic volume fraction reflecting oxygen (O_2) availability in combination with temperature and moisture effects. Further, it incorporates explicit diffusion of gaseous N compounds and O_2 through soil layers and to/from atmosphere. The gas diffusivity is largely influenced by *d_eff_reduction*, which remained close to the default value across sites (Fig. 2). This representation of gas transport is of importance since emissions of denitrification products can be delayed under anaerobic conditions by being entrapped within the soil at high soil moisture levels, hindering diffusion (Ding et al., 2022). Some versions of APSIM have implemented a retardation function to replicate these delays between gas production and emissions of denitrification products (Mielenz et al., 2016). Gas diffusivity also affects the product ratio between N_2O and N_2 (Balaine et al., 2016), which is reflected in model parameters like *dnit_k1* in APSIM. This parameter was found to be highly influential on N_2O emissions (Fig. 1) and differed between sites (Fig. 2), while currently assumed to be static and estimated coarsely by soil texture type. These findings on the calibration of parameters associated with gas diffusivity highlight that improved approaches to gas transport in soil may benefit an accurate simulation of N_2O and N_2 production and emissions from soils (Brilli et al., 2017).

The product ratio between N_2O and N_2 also shifts towards N_2O in response to increasing NO_3^- availability, as NO_3^- is preferred over N_2O as an electron acceptor for reduction by denitrifiers (Bizimana et al., 2021; Senbayram et al., 2019, 2012). The effect of NO_3^- on the product ratio is explicitly described in relation to C availability in APSIM. In LDNDC, the preference of the most abundant N-species is independent of the carbon availability. In the field, this effect was apparent at the Mackay site where the stool splitting application of N fertiliser on the cane row likely created zones of high NO_3^- concentration, compared to the Burdekin site with two-sided banding of N fertiliser (Takeda et al., 2022). Banding application of N fertiliser is known to slow hydrolysis of urea and inhibit nitrification (Janke et al., 2019, 2020), affecting substrate availability for denitrifying microbes after fertilisation. Fertiliser banding is a common practice in Australia, but the one-dimensional nature of APSIM and LDNDC does not fully account for these effects. Improved representation of local N cycling and its scaling to the conventional plot scale are an important challenge in common with many other biogeochemical models.

Another factor known to be influential on the product ratio between N_2O and N_2 while not accounted for in the current version of the models is soil pH, which inhibits reduction of N_2O to N_2 under acidic conditions (Dannenmann et al., 2008; Russenes et al., 2016; Šimek and Cooper, 2002). This pH effect, often reported in the range of 4.0–7.0, may explain the difference in magnitude of N_2O emissions between sites (Takeda et al., 2022) and also the greater discrepancy between observed and simulated N_2O emissions at the Mackay site (pH: 4.1) compared to the Burdekin site (pH: 6.9) (Fig. 5). Other models such as SWAT (Wagena et al., 2017) and DayCent (Blanc-Betes et al., 2021) have accounted for the pH effects on the denitrification and its product ratio and improved simulation of N_2O emissions. These simulation exercises of the present and previous studies indicate the potential to improve estimation of denitrification losses with more generic parameters across soil conditions by introducing such pH functions into APSIM and LDNDC.

Our findings from the site-specific fitting of these biogeochemical models to two distinct sugarcane systems highlighted the key challenges of applying the models across the Australian sugar industry or to diverse cropping systems. This modelling exercise illustrates the space to further improve denitrification algorithms and constrain N cycling of the models with both N_2O and N_2 across different soil types and pH to account for the factors discussed with generic parameter sets.

4.3. Implications of N budget comparison across calibrations, sites and models

The calibration of denitrification related parameters did not substantially alter the plant N uptake or overall N budget. However, the different calibration strategies did lead to a shift in N loss pathways, mainly between leaching and denitrification (Fig. 6). The models calibrated with both N_2O and N_2 showed greater denitrification losses compared to the models calibrated with N_2O only. This shift likely occurred because the denitrification process consumed available NO_3^- in the system, reducing the amount available for leaching. Furthermore, the simulated N budgets demonstrated a better agreement between the models when N_2 data is used in calibration (Fig. 6). Therefore, the findings of this study indicate the potential bias in assessments of N budget when the models are fitted to N_2O only and emphasise the critical role of N_2 emission data to constrain N cycling in biogeochemical models.

The models calibrated with field-measured N_2O and N_2 demonstrated the significance of denitrification, predominantly as N_2, as a pathway of N export from the sugarcane systems (Fig. 6). This corroborates the findings of the previous field study identifying the proportion of denitrification as > 30 % of fertiliser ^{15}N loss (Takeda et al., 2023). Such information on N_2 emissions and the N budget is often not provided in the majority of modelling studies reporting validation and projection of N_2O emissions (Grosz et al., 2023), which usually accounts for less than 5 % of N losses in most agroecosystems including this study. Information on the model's representation of the complete N budget is critical not only for evaluation of N_2O emissions but also point out knowledge gaps and ensure that the measured N fluxes are not matched by models for the wrong reasons (Grosz et al., 2023). For example, the evaluation of dissolved inorganic N exports to the Great Barrier Reef is currently done using APSIM (McCloskey et al., 2021), and this assessment would be significantly affected by the calibration of the denitrification sub-model, which alters the balance between N loss pathways. Reporting not only N_2O but also N_2 and the simulated N budget provides valuable insights into the model's representation of N cycling for subsequent simulation studies adapting the calibrated model and parameters with a broader scope.

The simulated N budgets reveal a potential risk of N mining at the Burdekin site with burnt trash management and N sequestration at Mackay with GCTB practice (Fig. 6). The balance between N inputs and exports did not improve by increasing N fertiliser rates, which is in agreeing field studies using fertiliser ^{15}N mass balance (Takeda et al., 2022, 2021b). The simulated N balance highlighted that trash management practices are critical for long-term N retention and thus soil carbon stocks, corroborating the previous modelling study in the wet tropics (Meier and Thorburn, 2016). Therefore, these findings support the recommendations to retain sugarcane trash instead of burning for a sustainable soil management practice.

This site difference in the overall N budget was demonstrated by both models with consistent denitrification losses after calibration with both N_2O and N_2 data. Nevertheless, APSIM demonstrated a greater difference in the sum of N export between the two sites with different trash management strategies (i.e. burnt trash management at the Burdekin site and trash blanket management at the Mackay site) compared to LDNDC (Fig. 6). This is partially due to the difference in simulated plant N uptake and its return to the soil, but also the difference in N supply via mineralisation and/or residue decomposition between the models. Several N cycling processes are explicitly described only in one model and not in the other, such as N runoff (only in APSIM), NO emissions (only in LDNDC), NH_3 volatilisation (only in LDNDC), though these processes had negligible impacts on the total N budget in this study (Fig. 6). Nevertheless, these N cycling processes may become influential under different soil and climate conditions and farming practices such as fertiliser application methods. Further inter-model comparisons as demonstrated in the present study and also ensemble modelling approaches can help harmonize the representation of N cycling in biogeochemical models.

5. Conclusions

This study demonstrated that while the calibration with N_2O data alone can improve simulation of N_2O emissions, it might compromise the simulation of agronomically significant N_2 emissions in APSIM and LandscapeDNDC. These findings underscore the critical importance of utilizing both N_2O and N_2 data to effectively constrain biogeochemical models to simultaneously simulate denitrification losses and improve N budget estimates. This is of particular importance when assessing the environmental impact of agricultural systems since underestimating environmentally benign N_2 emissions may lead to incorrect estimates of environmentally harmful reactive N losses in the form of N_2O emissions or NO_3^- leaching. This uncertainty in the model shifting N loss pathways between reactive N and inert N_2 potentially result in severe consequences for the farming community. The simulated N budgets unveiled potential concerns related to N mining from the burning of sugarcane residues compared to their retention. Interestingly, increasing N fertilizer rates did not improve the N balance in the system with trash burning. Furthermore, the comparison between models and sites has revealed opportunities for potential enhancements in denitrification algorithms within biogeochemical models, such as gas transports and pH responses. The findings of this study highlight the need for incorporation of laboratory and field experimental data on both N_2O and N_2 emissions under a broader range of conditions into biogeochemical models to reduce uncertainty in N budget estimates in future studies.

CRediT authorship contribution statement

Clemens Scheer: Writing – review & editing, Supervision, Funding acquisition. **Peter Grace:** Writing – review & editing, Supervision, Project administration, Funding acquisition. **Edwin Haas:** Software, Resources. **David Kraus:** Writing – review & editing, Software, Resources. **Johannes Friedl:** Writing – review & editing, Supervision, Project administration. **David Rowlings:** Writing – review & editing, Supervision. **Naoya Takeda:** Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

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.

Data Availability

Data will be made available on request.

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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.agee.2024.109193.

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