Journal of Cleaner Production 486 (2025) 144479

Contents lists available at ScienceDirect

Journal of Cleaner Production

journal homepage: www.elsevier.com/locate/jclepro

An integral assessment of carbon and nitrogen emissions in dairy cattle production systems: Comparing dynamic process-based greenhouse gas emissions factors with IPCC Tier 1 and Tier 2 approaches in confinement and pasture-based systems

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ARTICLE INFO

Handling Editor: Yutao Wang

Keywords:
Dairy cattle
Biogeochemical models
IPCC methodology
Manure-DNDC
Model evaluation
Tier 3 approach

ABSTRACT

The assessment of greenhouse gases (GHG) and nitrogen (N) emissions is essential for climate change mitigation. The Intergovernmental Panel on Climate Change (IPCC) provides guidelines for GHG quantification at both national and global levels. However, the IPCC Tier 1 (T1) and Tier 2 (T2) estimates, mostly used in national inventories, rely on generic emission factors (EFs) and empirical equations that are not suitable for case-specific assessments on individual farms. Thus, a more advanced Tier 3 (T3) methodology is needed to reflect the impact of key factors on emissions and reveal the effect of emission mitigation measures. Here we compare the IPCC T1 and T2 estimates to results from a cascade of process-based (PB) models referred to as T3 approach, for farm-level emissions. The results showed that the estimates from PB models differ significantly from those of the IPCC T1 and T2 estimates and allow more capability to predict variation. Moreover, PB models account for temporal changes and the underlying mechanisms responsible for GHG and N emissions. These models can be adopted for case-specific GHG assessment and project future mitigation strategies under different climate scenarios, regional contexts and on-farm management. Additional to the known applicability of PB models to estimate enteric methane (CH_4)and soil emissions, the present study demonstrates for the first time in Germany and Europe the effectiveness of Manure-DNDC model in simulating ammonia (NH_3) and CH_4 barn emissions, highlighting the potential for using PB models in case-specific GHG and N assessments for the whole manure management chain. Overall, this study presents options for a methodology in case-specific GHG assessment that can capture the effect of climate change and mitigation measures.

1. Introduction

Climate change induced by greenhouse gas (GHG) emissions is one of the most urgent challenges of our time (IPCC, 2023). The dairy cattle industry is a significant contributor to GHG and nitrogen (N) emissions, accounting for approximately 4% of total anthropogenic GHG emissions,

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https://doi.org/10.1016/j.jclepro.2024.144479
Received 14 April 2024; Received in revised form 2 December 2024; Accepted 12 December 2024
Available online 13 December 2024

and about 20% of emissions within the agricultural sector (FAO, 2019). Enteric fermentation and manure management are the primary sources (Chang et al., 2021). To implement efficient mitigation strategies, accurate quantification of these emissions is essential.

Direct measurement of emissions according to appropriate protocols is expensive and sometimes technically difficult to implement. The emissions are often too variable to capture with this type of measurement, with a reasonable amount of measurement time. Following a modelling approach may be a better and more feasible path to follow. The choice of model and mathematical approach to follow depends on the objectives of the modelling exercise, the complexity to capture, and the scale at which it is to be applied (farm, regional or national level). Furthermore, the value of modelling individual emission sources is restricted until these models are combined to assess complete production systems. Interactions between these sources introduce complexities, emphasizing that the entire system is more than its parts. Indeed, feeding and management practices impact various processes differently, underscoring the need for a comprehensive assessment to accurately quantify total farm emissions (Rotz, 2018). Various models have been used to assess GHG and N emissions at different levels of the manure management chain (Ouatahar et al., 2021). Generally, less complex models are used in national inventories with generic or even constant emission factors (EFs), referred to as T1 [1] and T2 [2] approaches. They are generally adopted with activity data or farm data as key variables (e.g., animal population, fertilizer amount, manure storage type, pasture/crop type). Whole farm models or product-based life cycle assessment (LCA), which still need a broader level of standardization (Baldini et al., 2017), also typically use static approaches, such as EFs or empirical equations, which allow quantifying the emissions associated with an activity, but not for capturing the underlying biotic and abiotic processes.

Such modelling approaches are not meant to capture temporal and spatial variation in production systems, or to differentiate between the various conditions at which these processes occur. Therefore, these EFs fail to capture the impact of, for example, the level of feed intake, feed composition and feed digestibility, the characteristics and quantity of animal waste during storage and handling, or the impact of soil type and conditions, as well as environmental factors affecting the production of gaseous emissions from farm facilities (Li et al., 2012). Also, addressing the variation in efficacy of various mitigation measures warrant improved accuracy and representation of the order of mitigation achieved (irrespective of variability encountered) and its potential trade-offs and synergies. Hence, adopting more advanced T3 methodologies when assessing emissions should provide more accurate estimates of GHG and N emissions, including their changes at the farm and national scale. Tier 3 methods involve the use of country-specific strategies, including detailed inventory measurements and process models (IPCC, 2006). In literature, the T3 method encompasses a range of models, from empirical to static mechanistic models, to dynamic mechanistic models, also referred to as 'process-based' (PB) models (Ouatahar et al., 2021).

Process-based simulation models that simulate emissions from different farm components or emitting processes, such as digestion, animal metabolism and production (Rotz et al., 2021) animal housing, manure storage and application to soil (Amon et al., 2021), including their biotic and abiotic drivers, would fall within the T3 category of IPCC system of inventory methodology (IPCC, 2019a). Process-based models capture the dynamics of carbon (C) and N fluxes, crucial for assessing mitigation strategies and projecting emissions. This enables a comprehensive whole-farm budget of GHG and N emissions within specific systems (Veltman et al., 2017). Ensemble modelling, where multiple PB frameworks are linked (Beukes et al., 2011), provides an integrated assessment of how dietary changes or manure storage affect emissions downstream the manure management chain, though this approach remains underutilized (Ouatahar et al., 2021).

The development and adoption of these approaches is particularly relevant, where 'carbon farming' or domestic offsetting schemes require accurate farm or field level quantification of emissions and proposed mitigation measures' reduction potential, requiring effective Measurement, Reporting, and Verification (MRV) strategies (UNFCCC, 2014). This also maximizes the efficacy of agricultural marginal abatement cost curve efforts (Eory et al., 2018).

The aim of this study is to compare a comprehensive PB modelling approach, referred to as the T3 methodology, with the simpler IPCC T1 and T2 methods across various stages of the manure management chain. This includes animal production, housing, manure management, and soil application (e.g., manure application and fertilization). Furthermore, the study evaluates the effectiveness of the Manure-DNDC model in simulating barn GHG and ammonia (NH_3) emissions, focusing on the housing component. The results provide a better understanding of the potential and need for T3 methodology (PB models) to generate dynamic, case-specific EFs, which capture the variability in GHG and N emissions across different production systems. This contributes to addressing the challenges of properly accounting for mitigation effects and making integral assessments of GHG and N emissions at the farm scale, thus improving the alignment between national inventories and farm-level estimates.

2. Materials and methods

2.1. Case study farms

Data from two dairy farms are used as case studies, one in Germany (farm 1) and the other in New Zealand (farm 2). Farm 1 is a naturally ventilated confinement system located in Groβ Kreutz, Germany, with an area of 905 ha and a herd of 235 Holstein cows. The soil is loamy sand, and mineral and manure fertilization are applied to the field. An anaerobic mesophilic biogas system and slurry tanks are used for manure management. Farm 2 is a pasture-based farm system located in Waikato, New Zealand, with 18 ha and a herd of 42 Holstein cows and 19 heifers. This farm system was one of four New Zealand regional farm systems designed to develop system-level solutions for profitably increasing production while reducing N leaching (Beukes et al., 2017). The soil at this Waikato farm trial is silt-loam with applied mineral fertilization. The case studies differ significantly in terms of farming intensity, fertilization intensity (kg of N ha^{-1} $year^{-1}$), and feeding intensity (DM intake and milk yield, kg cow^{-1} $year^{-1}$).

2.2. Tier 3 methodology: the cascade of process-based models

2.2.1. Modelling approach

The methodology employed in this study consists of a multi-step process that integrates a cascade of PB models to assess the impact of diet and manure management on GHG and N emissions from two case study dairy cattle systems. The modelling approach consists of three key components: the animal model, the housing and manure storage model, and the soil model. Each component captures distinct stages of emissions and nutrient flows throughout the farm system.

The simulation period for the confinement system (Farm 1) was 2018–2019 (one-year simulation). The herd was divided into categories with distinct DMI and milk characteristics, live weights, % crude protein (CP), DM fraction, and days in milk (DIM). This approach accounts for the variation between different animals in the herd, specifically categorizing them into high and mid-lactating cows, late-lactating cows, and dry cows. For the pasture-based system at Farm 2 in New Zealand, a

[1] T1 is considered the simplest method that could be standardized across countries for a subcategory called T1a that is more suitable for countries that have their production systems split up into low and high productivity systems for example, but detailed aspects of farming are lacking.

[2] T2 are EFs using variables that represent aspects of farming systems specific to each country (e.g., enteric CH_4 emission as a function of gross energy intake).

four-year simulation (2012–2015) was conducted for dairy cows, with an additional one-year simulation for heifers. This longer simulation period was chosen to capture the interannual variation inherent in a pasture-based system. By selecting these distinct monitoring periods and farming conditions, the aim was to demonstrate how PB models can effectively capture and differentiate the variability in GHG and N emissions across diverse agricultural practices.

The interdependence of dietary effects on GHG emission sources and the various components of the farm was investigated through the exchange of inputs and outputs between PB models. These steps allow for a comprehensive assessment of the downstream impacts of diet and manure management on GHG and N emissions, providing dynamic, case-specific EFs that reflect the temporal and spatial variations within the farm system. Fig. 1 provides a detailed visualization of the overall process, highlighting the inputs, outputs, and connectivity of each step in the modelling cascade.

The models were parameterized and calibrated using the site-specific data for animal, feed, housing, manure management, climate, soil, and crop/grass production. Crop parameters for crops and grass were adjusted to reflect the measured maximum yields and the length of Germany's and New Zealand's growing season. Due to the lack of detailed information on C pools, a 20-year spin-up run was conducted based on the known long-term land use history to achieve balanced C pools (Zimmermann et al., 2018). Standard preset values were used for unknown soil and crop parameters.

The main input data comprising feed information, housing, manure storage, climate (indoor and outdoor), land management and soil characteristics is presented in appendix A, and further assumptions of the modelling process are presented in appendix B (Table B2).

2.2.2. Steps of the modelling process

2.2.2.1. Modelling enteric methane emissions. In the first step, the animal model (The Dutch Tier 3 model) was used, which is currently applied as a T3 approach (Bannink et al., 2011). This model simulates the impact of feed intake, chemical fractions in feed and rumen degradation characteristics of these chemical fractions on microbial activity in the rumen. Mills et al. (2001) incorporated additional equations describing the digestive processes in both the small and large intestine, and the process of enteric methanogenesis was included. Recently, the model was updated to improve the prediction of apparent fecal N and organic matter (OM) digestibility (Bannink et al., 2018) and excreta composition (Dijkstra et al., 2018). The model outputs include enteric CH_4 emissions, methane conversion factor (MCF), and N and C content in urine and feces, which serve as inputs for the next stage.

2.2.2.2. Modelling manure management emissions. In the second step, the housing and manure storage model (ManureDNDC) (Li et al., 2012) simulates GHG and N emissions from manure handling and storage. The model receives inputs from the animal model (i.e., N and C content in manure) and data on housing structures, and milk/diet chemical composition, along with the daily variations in surrounding abiotic housing and storage conditions, such as housing microclimate and manure removal frequency. The outputs of this stage include emissions of nitrous oxide (N_2O), CH_4, NH_3, nitrate (NO_3^-) and the volume of manure excreta.

Tier 3 VS (kg animal^{-1} year^{-1}) were estimated according to the empirical equations incorporated into the Manure-DNDC model (Appuhamy et al., 2018). The predictor variables were organic matter (OM) (kg d^{-1}), neutral detergent fiber (NDF) and CP contents (% of dry matter intake (DMI)):

$$VS = [-1.201 + 0.402 \times OM + 0.036 \times NDF - 0.024 \times CP] \times 365$$

Equation 1

Ultimately, the manure excreta arising from storage is spread on soil and thus enter the soils module of DNDC.

2.2.2.3. Modelling soil emissions and removals. The third step involves

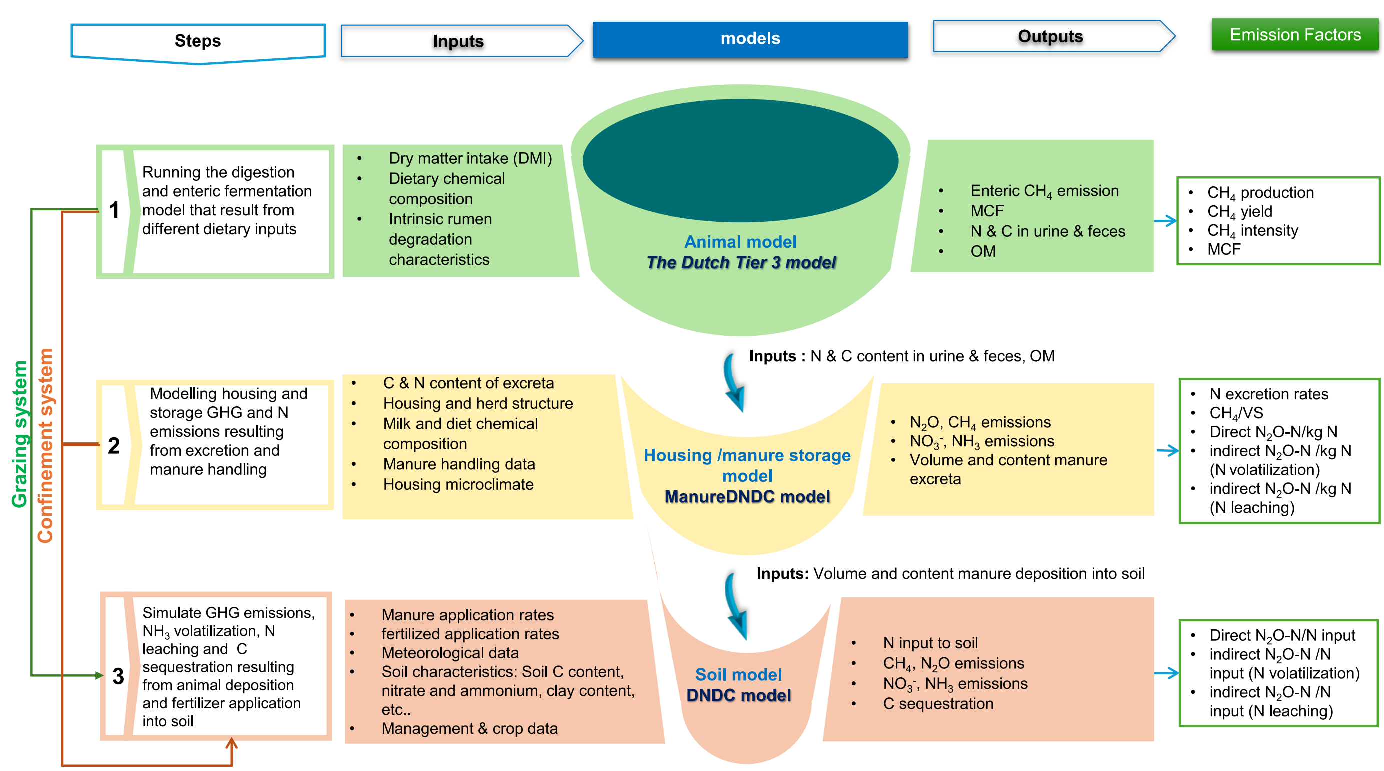

Fig. 1. Summary of the modelling steps, inputs data, outputs data, and the connectivity of each step of the modelling process using the cascade of process-based models (Tier 3). C: Carbon, N: Nitrogen, GHG: greenhouse gas, MCF: methane conversion factor, OM: organic matter, VS: volatile solids.

the soil model (DNDC model, v9.5) (Li et al., 1992a, 1992b), which simulates the emissions and nutrient fluxes that occur after manure application to the soil. Inputs for this model include manure and fertilizer application rates, meteorological data, and crop and soil characteristics. DNDC was originally developed to simulate soil C and N cycling (Li et al., 1992b). It gained popularity due to its detailed biochemical equations describing decomposition, nitrification and denitrification processes. It contains sub-models for simulating crop biomass, decomposition, nitrification, denitrification, fermentation and NH_3 volatilization, with abiotic drivers including climate and soil physico-chemical properties. As the model simulates a very wide array of agricultural management and crop types, DNDC has been used extensively worldwide (Gilhespy et al., 2014) with continuous improvement and calibration (Deng et al., 2020). In terms of GHGs, the model simulates both direct and indirect N_2O emissions (Giltrap et al., 2010), soil CH_4 and soil organic carbon (SOC) changes.

Indirect N_2O emissions were calculated for NH_3 volatilization ($N_2O\_indirect - N\ (NH_3)$) and N leaching ($N_2O\_indirect - N\ (NO_3^-)$) in kg year−1, assuming all lost N was locally redeposited, as follows:

$$N_2O_{indirect} - N\ (NH_3) = NH_3 - N \times EF_4 \quad \text{(Equation 2)}$$

$$N_2O_{indirect} - N\ (NO_{3^-}) = NO_{3^-} - N \times EF_5 \quad \text{(Equation 3)}$$

EF_4 (0.01) and EF_5 (0.011) are IPCC EFs for N_2O emissions from NH_3 volatilization and NO_3^- leaching, respectively (IPCC, 2006a; 2019).

2.3. IPCC tier 1 and tier 2 methodology

DMI and chemical composition of the diets were collected from activity data and used as input for the PB models. For the T2 calculations related to the enteric CH_4, DMI was estimated according to IPCC (IPCC, 2019a):

For cows: DMI = 0.0185 × BW + 0.305 × FPCM (Equation (4)).

For heifers: DMI = 3.184 + 0.01536 × BW × 0.96 (Equation (5)).

Where BW is body live weight in kg animal^{-1} and FPCM is fat protein corrected milk in kg day^{-1}.

Gross energy (GE, MJ day^{-1}) was estimated as follows according to the IPCC methodology for the T2 calculations (IPCC, 2019a):

$$GE = \left[\left(\frac{NE_m + NE_a + NE_l + NE_p}{REM}\right) + \left(\frac{NE_g}{REG}\right)\right] \Big/ DE \quad \text{(Equation 6)}$$

Where NE_m is net energy required by the animal for maintenance, NE_a is net energy for animal activity, Ne_l is net energy for lactation, NE_p is net energy required for pregnancy, REM is the ratio of net energy available in a diet for maintenance to digestible energy, NE_g = net energy needed for growth, REG = ratio of net energy available for growth in a diet to digestible energy consumed, DE = digestibility of feed expressed as a fraction of gross energy (digestible energy/gross energy).

Average N excretion (kg N animal^{-1} year^{-1}) according to T1 methodology was calculated as follows (IPCC, 2019a):

$$Nexcretion = \left(N_{rate} \times \frac{TAM}{1000}\right) \times 365 \quad \text{(Equation 7)}$$

N_{rate} is default N excretion rate, (kg N (1000 kg animal mass)$^{-1}$ day$^{-1)}$, and TAM is typical animal mass (kg animal^{-1}). A TAM of 600 and 488 was assumed for the dairy cows in the confinement and pasture-based system respectively. For heifers, 389 was considered (IPCC, 2019a).

Volatile solids (VS) (kg year^{-1}) according to T1 methodology were estimated as follows (IPCC, 2019a):

$$VS = \left(VS_{rate} \times \frac{TAM}{1000}\right) \times 365 \quad \text{Equation 8}$$

Where VS_{rate} is the default VS excretion rate, and TAM is typical animal mass.

Table 1 gives an overview of the outcome for the main mass flow variables and associated EFs when following the IPCC T1 or T2 methodology.

Given that this study does not compare T3 estimates with inventories, we did not calculate case-specific N excretion rates or VS for the two case studies using a T2 approach.

2.4. Evaluation of Manure-DNDC model

2.4.1. Model evaluation against measured data

Daily and cumulative modelled fluxes with Manure-DNDC were evaluated against measured CH_4 and NH_3 fluxes inside the barn of lactating dairy cows for the corresponding monitoring period in the confinement system. Such evaluations were essentially lacking for this PB model in previous studies in the European context for barn emissions (in contrast to the other PB models used). Hence, model applicability had to be studied before comparing PB model simulations on GHG and N emissions with T1 and T2 methodology. The measurements were conducted using the carbon dioxide (CO_2) balance method for 36 consecutive days (from January 24, 2018 to February 28, 2018), using a Fourier-Transform Infrared (FTIR) gas analyzer, and following the sampling procedure of the VERA protocol (VERA, 2018). Previous studies describe the sampling (Janke et al., 2020) and measurement protocol (Bobrowski et al., 2021) in detail. The coefficient of determination (R^2) and root mean square error (RMSE) were calculated to evaluate the model's accuracy.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Pi - Oi)^2}{n}} \quad \text{(Equation 9)}$$

Where Pi is predicted values by the model, and Oi are observed values from on-site measurements in the barn, and n is the number of observations. The relative RMSE is calculated by dividing the RMSE by means of the observed values.

For testing the statistical significance associated with observed correlations, we used the Pearson correlation test, and employed the quantile mapping approach (Volosciuk et al., 2017) for statistical bias correction (Piani et al., 2010), assuming a linear bias and thus implementing a linear regression model to obtain the transfer function for the bias correction expressed as:

$$E_{obs-sorted} = A * E_{mod-sorted} + B. \quad \text{(Equation 10)}$$

Here $E_{obs\text{-}sorted}$ refers to datasets of observed CH_4 and NH_3 emission values from measurement campaigns. The values in each of the datasets have been sorted independently from lowest to highest value. Similarly, $E_{mod\text{-}sorted}$ refer to the data sets of modelled CH_4 and NH_3 emissions values, which have also been sorted in ascending order. A is the slope of the line, and B is the intercept. This approach facilitates the estimation of statistical bias in both the mean and variance of simulations relative to the measured values. The intercept of the transfer function reflects the mean bias (zero indicating no bias), while the slope indicates the variance bias (one denotes no bias).

2.4.2. Model sensitivity

To investigate the behaviors of the housing component of Manure-DNDC, sensitivity tests were conducted by varying key input parameters. For animal/diet parameters, adjustments were made to the feed rate, %CP in the diet, and DIM. For housing and manure management, variations included barn temperature, barn surface area, and manure removal frequency. The baseline scenario was based on actual conditions, while alternative scenarios were created by varying one input parameter at a time, keeping others constant (Saltelli and Annoni, 2010). The sensitivity of modelled barn floor NH_3 and CH_4 emissions to the input parameters was expressed with the sensitivity index (SI)

Table 1
Mass flow variables and emission factors following IPCC Tier 1 (T1) or Tier 2 (T2) methodology in assessment of GHG and N emissions in a confinement system (farm 1) and a pasture-based system (farm 2).

Farm component	animal category/Tier	Type of direct/indirect GHG	Emission factor	unit	farm 1	farm 2	reference
Animal	Dairy cows T1	enteric CH_4	CH_4 production	kg head^{-1}	126.0	93.0	(IPCC, 2019a), table 10.11
	Heifers T1	enteric CH_4	CH_4 production	kg head^{-1}		63.0	(IPCC, 2019a), table 10.11
	dairy cows T1	enteric CH_4	CH_4 yield	g/kg DM	20.0	21.4	(IPCC, 2019a), table 10.12
	Heifers T1	enteric CH_4	CH_4 yield	g/kg DM		23.3	(IPCC, 2019a), table 10.12
	Dairy cows T2	enteric CH_4	MCF	%GEI	6.0	6.5	(IPCC, 2019a), table 10.12
	Heifers T2	enteric CH_4	MCF	%GEI		7.0	(IPCC, 2019a), table 10.12
Housing and manure management	Dairy cows T1	CH_4	EF_{TSP}	kg CH_4 kg Vs^{-1}	22.5		(IPCC, 2019a), table 10.14
	Dairy cows T2	CH_4	B_0	m^3 CH_4 kg^{-1} VS	0.24		(IPCC, 2019a), table 10.16
	Dairy cows T1	N excretion rate	N excretion rate	kg N (1000 kg animal mass)$^{-1}$ day-^{1}	0.50		(IPCC, 2019a), table 10.19
		N_2O	EF_3	kg N_2O-N/kg N	0.005		(IPCC, 2019a), table 10.21
		N_2O	FracGasMS	kg N_2O-N/kg N	0.48		(IPCC, 2019a), table 10.22
		NH_3	EF_4	kg N_2O-N/kg N	0.01		(IPCC, 2019a), table 11.3
Soil	T1	N_2O	EF_1	kg N_2O-N/kg N	0.01	0.01	(IPCC, 2019b), table 11.1
	T1	N_2O	EF_{3PRP}	kg N_2O-N/kg N	0.004	0.004	(IPCC, 2019b), table 11.1
	T1	NH_3	EF_4	kgN_2O-N/kg N	0.01	0.01	(IPCC, 2019b), table 11.3
	T1	NO_3^-	EF_5	kgN_2O-N/kg N	0.011	0.011	(IPCC, 2019b), table 11.3

N: nitrogen, GHG: greenhouse gas; VS: volatile solids, N_2O: nitrous oxide, CH_4: methane, NH_3: ammonia, NO_3^-: nitrate leaching, MCF: methane conversion factor, GEI: gross energy intake, EF_1: emission factor for direct N_2O emissions from N inputs to cultivated soils, EF_{TSP}: emission factor for direct CH_4 emissions from manure management, B_0: maximum CH_4 producing capacity for manure, EF_3: emission factor for direct N_2O emissions from the manure management system, $EF3_{PRP}$: emission factor for N_2O emissions from urine and dung N deposited on pasture, range and paddock by grazing animals, EF_4: emission factor for N_2O emissions from atmospheric deposition of N on soils, EF_5: emission factor for N_2O emissions from N leaching and runoff, FracGasMS: the amount of managed manure N for a livestock category that is lost by volatilization in the manure management system.

(Werner et al., 2007):

$$SI = \left((O_2 - O_1) \,/\, O_{avg}\right) / \left((I_2 - I_1) \,/\, I_{avg}\right) \quad \text{(Equation 11)}$$

Where, I_1 and I_2 represent the minimum and maximum input values for a specific parameter, while I_{avg} is their average. Similarly, O_1 and O_2 are the model output values corresponding to I_1 and I_2, with O_{avg} being the average of O_1 and O_2. The higher the absolute value of the index, the greater the impact of the input parameter on the output.

3. Results

3.1. Comparison of process-based models and IPCC tier 1 and tier 2 outputs

The main objective was to demonstrate the comparison between PB model outcomes (T3) and IPCC T1 and T2 calculations, using a case study for a confined dairy system (in Germany) and a pasture-based system (in New Zealand) dairy system. The comparison did not include an assessment or comparison of the two countries' current inventories, but the focus was on using two distinct farm case studies. The dairy cattle industry is pivotal in both Germany (dairy global, 2023) and New Zealand (Aziz et al., 2019). Therefore, accurate quantification and mitigation of GHG emissions are essential for both countries to meet their climate goals.

3.1.1. Methane emissions from enteric fermentation

In the confinement system, T3/PB enteric CH_4 values were 14%–19% lower for lactating cows compared to T2 predictions. Interestingly, T3 EFs were similar to T1 estimates. However, for dry cows, T3 estimates were 48% lower than T1 and 9% higher than T2. For the pasture-based system, T3 estimates ranged from 109.2 to 124.0 kg CH_4 head^{-1} year^{-1} for cows and 82.4 kg CH_4 head^{-1} year^{-1} for heifers, consistently higher (17%–36% for cows and 26%–31% for heifers) than Tiers 1 or 2 (Fig. 2).

The T3 results in g CH_4 kg^{-1} DMI or kg milk differed by −10% to −15% from the default IPCC T1 CH_4 yield (20.0 kg CH_4 kg DMI^{-1}) in the confinement system, while only slightly higher (1–2%) than the default IPCC T1 (21.4 kg CH_4 kg DMI^{-1}) for the pasture-based system. The T3 model predicted that 5.00–5.56% of gross energy intake was emitted as CH_4 for confinement systems, which were 7%–17% lower compared to the estimates with the default MCF used in the T2 approach. The variation in MCF rates in the pasture-based system was 1%–3% higher for cows. The same trend goes for heifers, only 1% higher MCF was estimated using the T3 approach.

3.1.2. Annual average nitrogen excretion rates

Fig. 3 compares N excretion estimates for cows and heifers using T3 and T1 methodologies. T3 predicts higher N excretion in the pasture-based system, ranging from 15% to 36% for cows and 111% for heifers compared to T1. In the confinement system, differences in total N excretion were lower with T3, notably −19% for dry cows. Results suggest N excretion varies by lactation stage and DMI, with early lactating cows excreting the most N (HL), followed by late lactating cows (LL) and dry cows (DC) excreting the least.

3.1.3. Methane emissions from manure management

In the pasture-based system, there was no manure management, as it lacks housing and manure storage (animals were on pasture 24 h day^{-1}). Therefore, manure management emissions (CH_4 and N_2O) were estimated only for the confinement system.

Substantial differences were obtained for gCH_4 kg^{-1} VS from manure management under the three model Tiers (Fig. 4). While the T1 approach used default values for all categories of cows, the T2 method used default animal waste management systems for manure management systems, while VS excretion rates were based on T2 calculations. The T3 estimates range from +37% for high lactating cows to +71% for dry cows compared to T1, and between +48% and +84% compared to the T2 approach.

3.1.4. Direct and indirect nitrous oxide emissions from manure storage

Fig. 5 compares direct N_2O EFs (kg N_2O-N kg^{-1} N excreted) generated using the various model Tiers. Indirect N_2O emissions, resulting from N volatilization (indirect N_2O volatilization) and N leaching (indirect N_2O leaching) from manure management for the confinement system, were also simulated. The T3 model generated intermediate emission estimates compared to the high emissions using T1 and the low emissions using the T2 approach. Furthermore, volatilization was predicted to be a more significant contributor to indirect N_2O emissions than leaching with the T3, which is not distinguished from the T1 and 2 approaches.

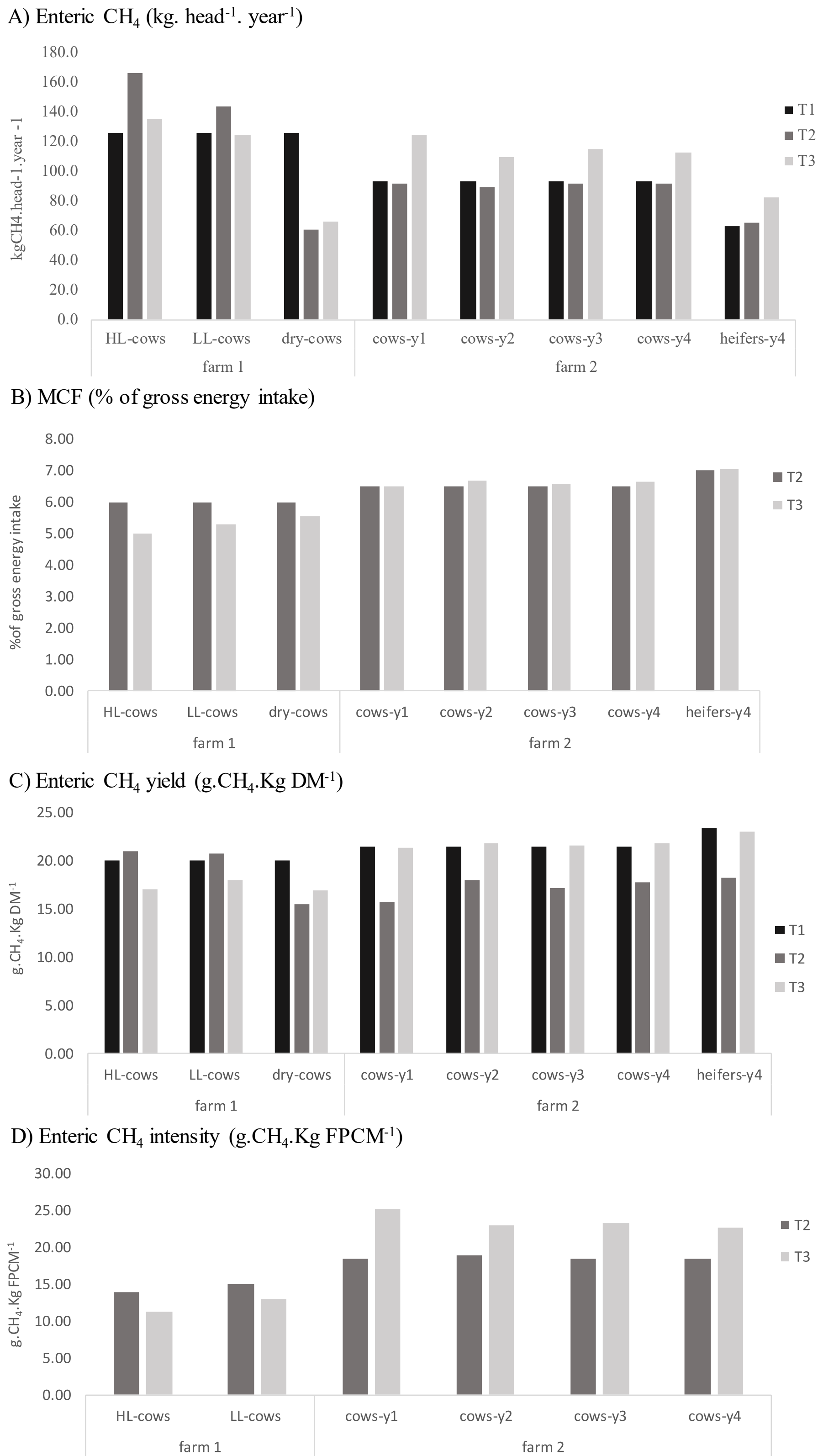

Fig. 2. Simulated enteric methane (CH_4) per cow. year^{-1} (kg), per DM intake (CH_4 yield), or per kg FPCM (CH_4 intensity), and CH_4 conversion factor (MCF) for both confinement system (farm1, Germany, one year simulation for different cows; HL-cows: high lactating cows, LL-cows: late lactating cows and dry cows) and for pasture-based system (farm 2, New Zealand, 4-year simulation for cows and one year for heifers; y1: year 1, y2: year 2, y3: year 3, y4: year 4).

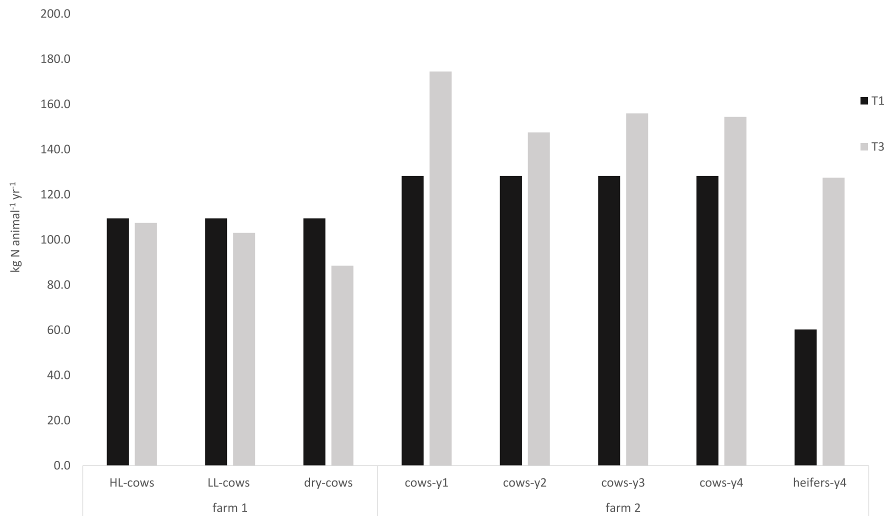

Fig. 3. Comparison of total nitrogen (N) excretion (kg N. head^{-1}. year $^{-1}$) estimated using the process-based model (T3) and Tier 1 (T1) methodology for both confinement system (farm1, Germany, one year simulation for different cows; HL-cows: high lactating cows, LL-cows: late lactating cows and dry cows) and for pasture-based system (farm 2, New Zealand, 4 year simulation for cows and one year for heifers; y1: year 1, y2: year 2, y3: year 3, y4: year 4).

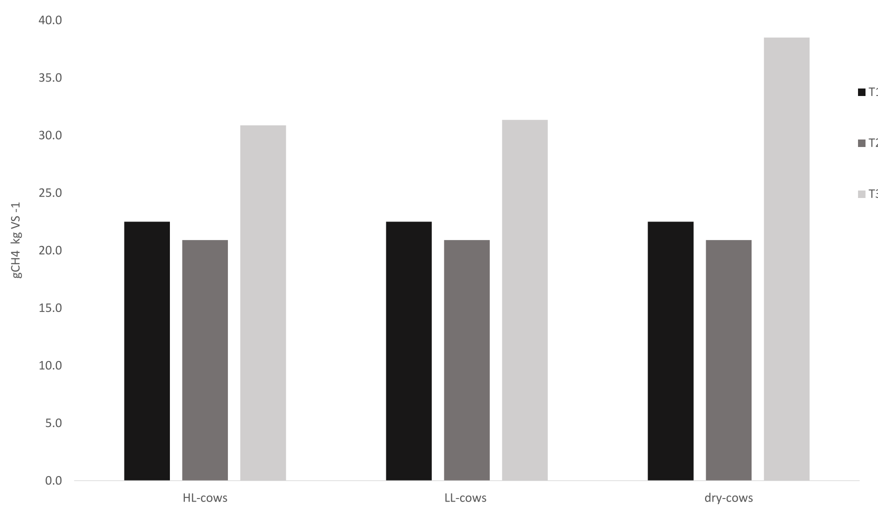

Fig. 4. Comparison of methane (CH_4) emissions per volatile solids excretion (VS), from manure, management for confinement system (farm1, Germany, one-year simulation for different cows; HL-cows: high lactating cows, LL-cows: late lactating cows and dry cows), T1: Tier 1, T2: Tier 2, T3: Tier 3.

3.1.5. *Direct and indirect nitrous oxide emissions from land application*

Direct N_2O emission rates estimated using the T1 method were substantially lower compared with emission rates generated using the T3 approach. In particular, direct N_2O emissions, using the PB approach, are two times higher than the generic T1 EF (i.e,. 1%) estimates for the confinement system. However, T1 estimates were 1.3 to 1.5 higher than T3 for the pasture-based system (Fig. 6).

Indirect soil emissions resulting from NO_3^- in the confinement system are also higher with the T3 model. All differences between the T1 and T3 calculations are largely driven by variations in soil physico-chemical properties (particularly soil texture), vegetation type and daily climate data, which were considered using the T3 approach, but were not captured by the static T1 EF approach. The T1 approach indicated that indirect N_2O emissions resulting from N volatilization and leaching dominated the confinement system and were higher compared to indirect emissions from the pasture-based system. Using the T3 approach, direct soil N_2O emissions comprised 62% of total N_2O emissions for the confinement system, and over 65–76% of N_2O emissions from the pasture-based system

3.2. *Evaluation and error analysis of the housing component of Manure–DNDC model*

The evaluation of Manure-DNDC's model in simulating CH_4 and NH_3 emissions inside the barn against measurement data metrics is summarized in Table 2. The comparison of simulated and measured daily and cumulative CH_4 and NH_3 emissions is shown in Fig. 7. Additionally, the scatter plots depicting the relationship between modelled and measured values for both daily and cumulative CH_4 and NH_3 emissions are provided in Fig. 8.

The models' performance was assessed using RMSE values, which indicate their proximity to observed data. For daily CH_4 fluxes, the RMSE value was 0.135 kg CH_4 head^{-1} day^{-1}, while for cumulative CH_4 fluxes, it was 1.153 kg CH_4 head^{-1}. Relative RMSE values, which highlight percentage-wise deviation, were 24.9% for daily CH_4 fluxes and 12.3% for cumulative CH_4 fluxes, indicating higher accuracy in the latter. Correlation analyses showed strong performance in cumulative CH_4 fluxes ($R^2 = 0.998$, Pearson correlation = 0.999), but weaker performance in daily CH_4 fluxes ($R^2 = 0.071$, Pearson correlation =

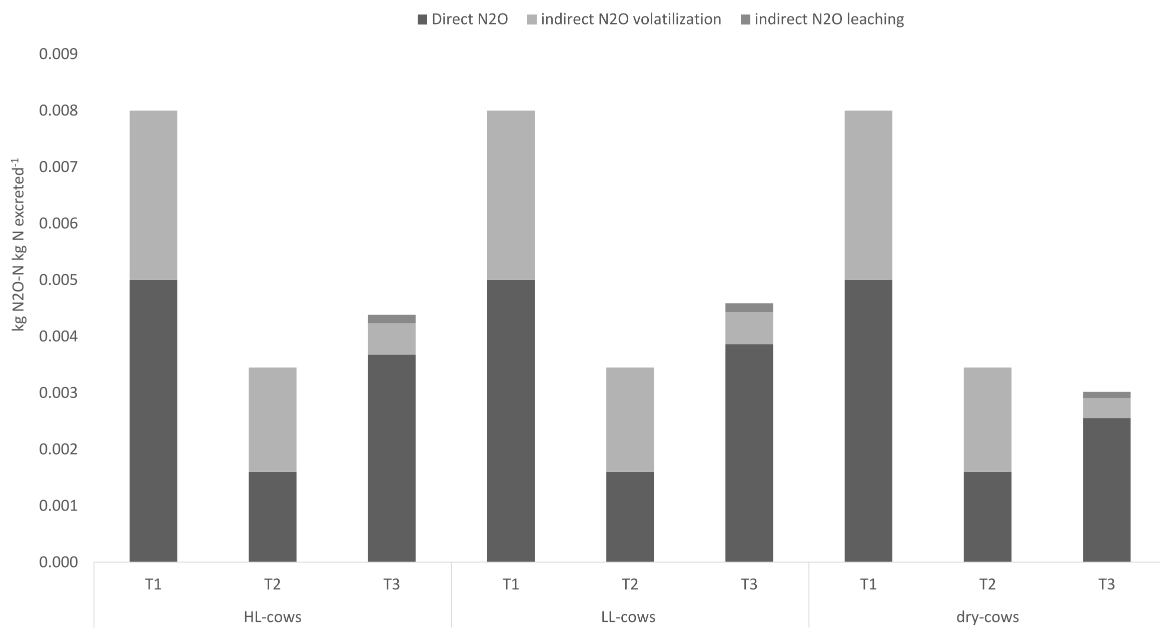

Fig. 5. Comparison of direct and indirect nitrous oxide (N_2O) per kg N excreted resulting from N volatilization (indirect N_2O volatilization) and N leaching (indirect N_2O leaching) from manure management for the confinement system (farm 1, Germany, one-year simulation for different cows; HL-cows: high lactating cows, LL-cows: late lactating cows and dry cows), T1: Tier 1, T2: Tier 2, T3: Tier 3.

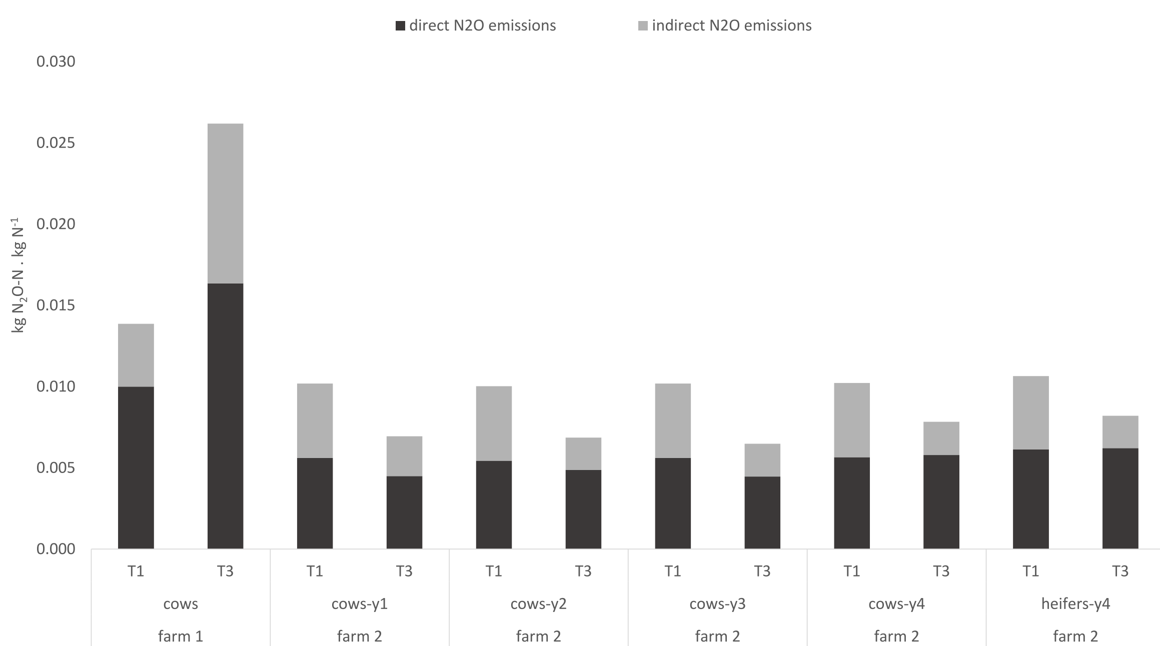

Fig. 6. Comparison of soil N_2O-N emissions per kg nitrogen (N) inputs for the total of direct and indirect N_2O emissions (N volatilization + N leaching) using Tier 1 (T1) emissions factors and Tier 3 (T3) modelling with DNDC model, for both the confinement system (farm 1, Germany, one year simulation for cows) and for the pasture-based system (farm 2, New Zealand, 4 year simulation for cows and one year for heifers areas; y1: year 1, y2: year 2, y3: year 3, y4: year 4). For Tier 3, indirect N_2O emissions were calculated using Tier 1 EF_4 and EF_5).

−0.266). Similar assessments for NH_3 emissions revealed an RMSE of 0.007 kg NH_3 head^{-1} day^{-1} for daily NH_3 fluxes and 0.043 for cumulative NH_3 fluxes. Relative RMSE values were 64.8% for daily NH_3 fluxes and 17.4% for cumulative NH_3 fluxes. Correlation analyses showed robust performance in cumulative NH_3 fluxes (R^2 = 0.998, Pearson correlation = 0.995), but weaker performance in daily NH_3 fluxes (R^2 = 0.107, Pearson correlation = 0.327).

The sensitivity analysis of Manure-DNDC model (Table B4; Appendix B), revealed that barn floor NH_3 and CH_4 emissions were highly responsive to changes in feed rate. CP content significantly impacted NH_3 emissions for dry cows. Additionally, barn temperature and manure removal frequency moderately affected CH_4 emissions within the test range, whilst DIM showed some sensitivity, primarily affecting NH_3 emissions. Barn surface area was negatively correlated with emissions,

Table 2
Summary of metrics for the error and bias test analysis for modelled CH_4 ($kgCH_4$ $head^{-1}$ day^{-1}) and NH_3 barn emissions ($kgNH_3$ $head^{-1}$ day^{-1}) using the Manure–DNDC model compared to measurement data.

Metric	Daily fluxes		Cumulative fluxes	
	Daily CH_4	Daily NH_3	Cumulative CH_4	Cumulative NH_3
Error analysis				
RMSE	0.135	0.007	1.153	0.043
Relative RMSE	0.249	0.648	0.123	0.174
Correlation analysis				
R^2	0.071	0.107	0.998	0.998
Pearson correlation	−0.266	0.327	0.999	0.995
correlation test – p-value	0.117	0.05187	<2.2e-16	<2.2e-16
bias test analysis - regression model				
p-value	<2.2e-16	4.78e-15	<2.2e-16	<2.2e-16
R^2	0.880	0.839	0.998	0.991
Intercept	−0.491	−0.002	−0.899	0.045
Slope	2.229	0.981	1.184	0.747

RMSE: root mean square error, CH_4: methane, NH_3: ammonia, R^2: coefficient of determination.

indicating that increasing space per animal reduced both NH_3 and CH_4 emissions.

4. Discussion

4.1. Comparison of IPCC emission factors and process-based models

At the farm level, the outputs generated using the T3/PB models clearly differed, compared to the T1 and T2 approaches, which are generally adopted in national inventories and many GHG assessment tools. These lower Tiers use static EFs, while the T3/PB model approach encompasses variations in biotic and abiotic drivers, such as feed quality, lactation stage, climate, manure storage length and soil type. Tier 3 approaches therefore capture the considerable variation in the dynamics in emissions that can occur on a more localized scale, such as variations between different seasons, years, soils, animal categories and farming systems. The findings align with those of Bannink et al. (2014), who assessed the impact of mitigation options across European farms using various PB models. Their comparison of T1, T2, and T3 approaches revealed significant differences in estimated enteric CH_4 and soil N_2O emissions. However, unlike the current study, they did not account for housing emissions. Furthermore, Ouatahar et al. (2024) assessed GHG and N emissions from dairy systems using PB models, with a focus on evaluating the impact of diet and manure management on whole farm emissions. However, the study did not evaluate the performance of the different IPCC-recommended methods for assessing farm-scale emissions. Building on this foundation, the present study advances the methodology by generating dynamic, case-specific T3 EFs and directly comparing them to the generic IPCC T1 and T2 approaches. This study provides a detailed comparison of T3 EFs with IPCC T1 and T2 methods and, by linking a cascade of process-based models, demonstrates the downstream effects of diet and manure management practices on GHG and N emissions. This whole-system approach offers a more comprehensive perspective than focusing on isolated stages of the manure management chain.

A study by Yan et al. (2010) found that the default factors of T1 for both enteric fermentation and manure management overestimated CH_4 emissions in dairy cows when compared to the EFs of T2 and T3 (the latter not including PB models as in the present study). Recently, Eugène et al. (2019) proposed a T3 methodology based on empirical equations to estimate CH_4 emissions inventory in France for ruminants concerning dietary information. Using this approach, estimates of enteric CH_4 were observed to be between 88% and 114% of the values for enteric CH_4 emissions provided by the IPCC methodology, with variation depending

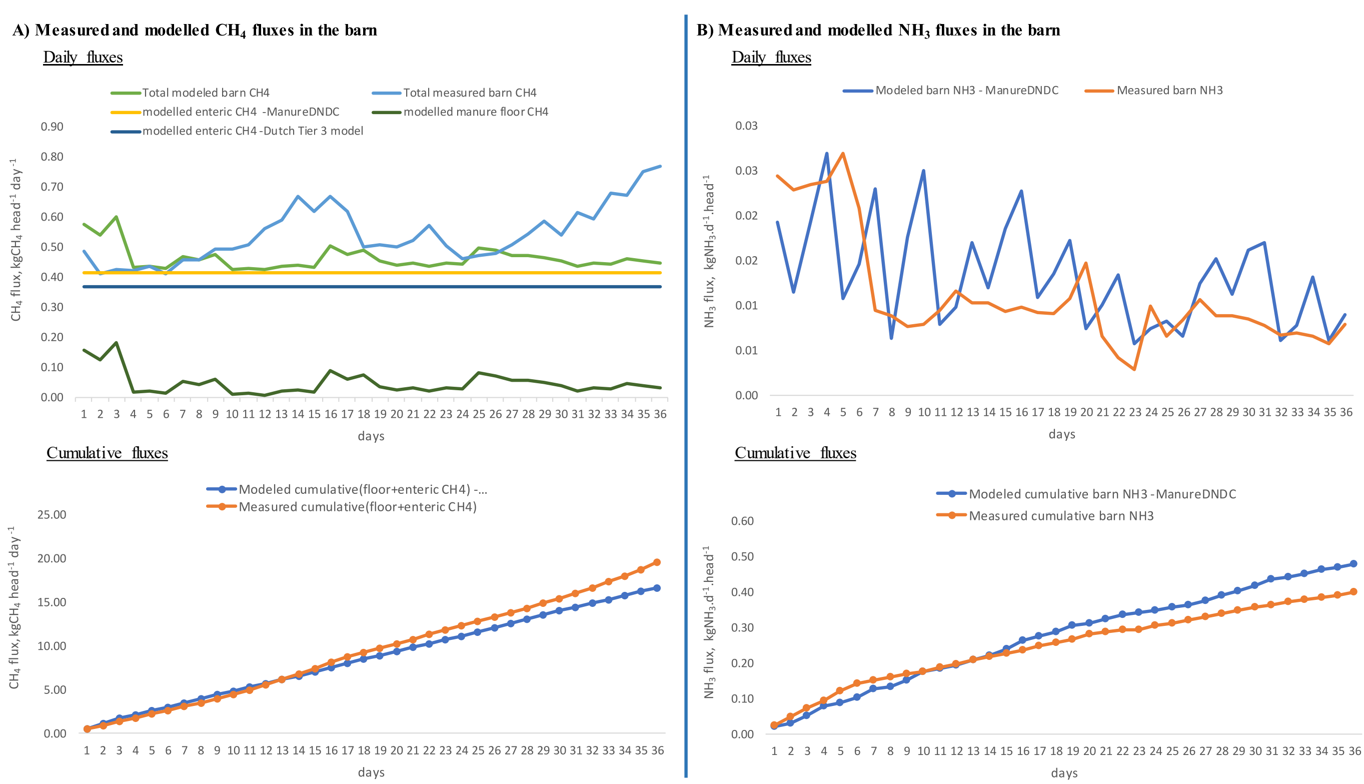

Fig. 7. Comparison between measured and modelled daily and cumulative emissions inside the barn in the confinement system A) total CH_4 (enteric + floor) using Manure-DNDC and B) NH_3 fluxes using Manure-DNDC. Modelled Enteric CH_4 was compared for both Manure-DNDC and the Dutch Tier 3 model in A). CH_4: methane, NH_3: ammonia.

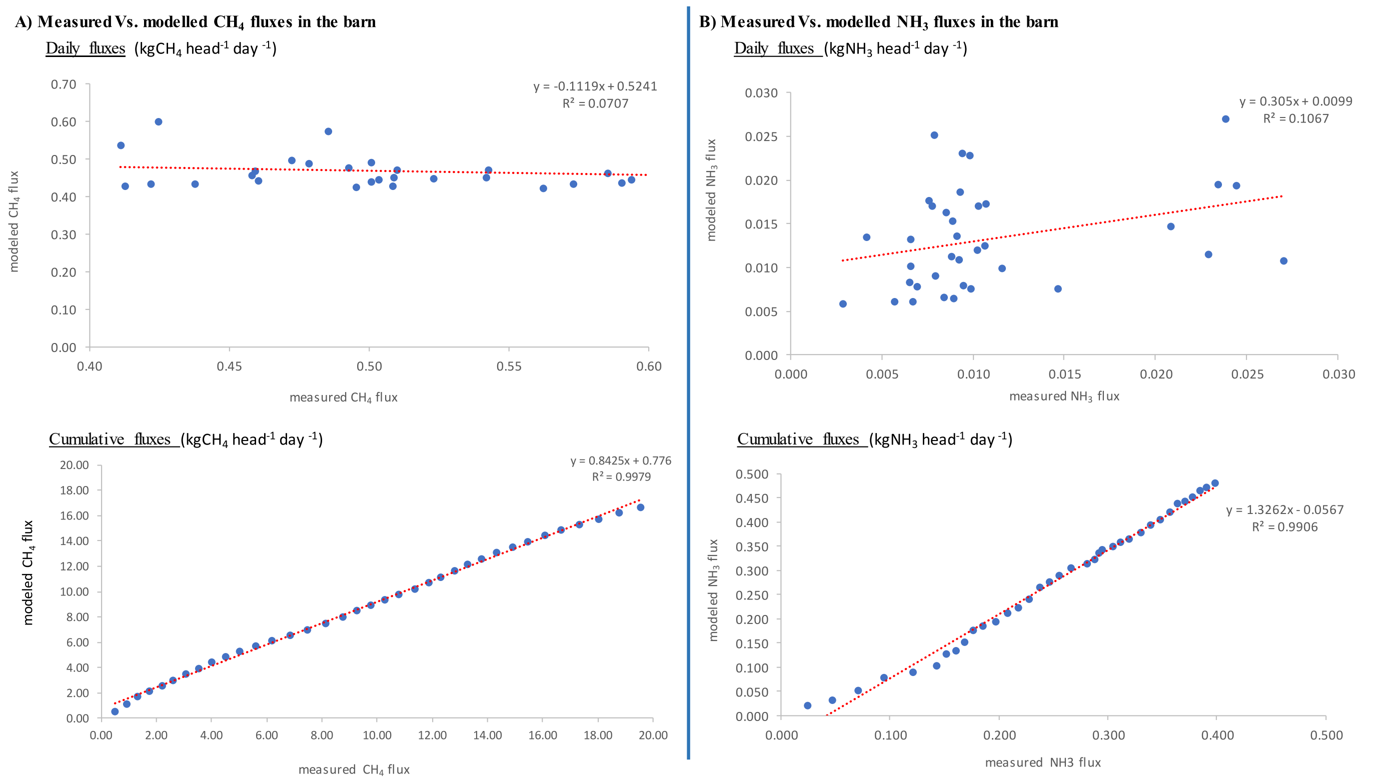

Fig. 8. Representation of the relationship between measured and modelled daily and cumulative methane (CH_4) and ammonia (NH_3) emissions inside the barn in the confinement system using Manure-DNDC A) total CH_4 (enteric + floor) and B) NH_3 fluxes.

on the animal category. The use of the rather static values with the lower Tiers for all categories of cows do not capture the differences due to DMI, production level of cows, chemical composition and digestibility of the diets. Accurate estimates of enteric CH_4 emissions in dairy cows require addressing rumen function's chemical and physical aspects through more complex models such as PB models. This aligns with the findings of Niu et al. (2018) who reported that the greater the complexity of the model, the better its ability to predict enteric CH_4 production. The models that best predicted CH_4 production were those that used DMI, NDF, crude fat, milk fat, and body weight in their complexity. Tier 3 approaches, especially those incorporating PB models, further enhance accuracy by addressing key biological processes, such as microbial activity, that simpler empirical models fail to capture.

The PB Dutch T3 model used in the present study as T3 approach has been used in the inventory of enteric CH_4 (Bannink et al., 2011) and NH_3 in the Netherlands (Dijkstra et al., 2018) and also requires such details as inputs, providing a CH_4 EF (kg CH_4 cow^{-1}year^{-1}) and the percentage of gross energy intake emitted as CH_4 as a predicted model outcome (in contrast to being an input or assumption as with the lower Tiers). It may also help develop and evaluate strategies for reducing GHG emissions from the dairy industry.

Predicted manure management emissions also depended on the chosen modelling approach. Manure-DNDC, as a PB model/T3 approach, predicts VS in relation to OMI, NDF and CP (Appuhamy et al., 2018), while T1 or T2 approaches use default values, which result in different predictions of B_0, the manure CH_4 production potential. In addition, the PB model generated housing/storage CH_4 and NH_3 emissions that were driven by climatic factors, such as temperature and wind speed (which governs the barn ventilation rates and surface evaporation rates), as well as manure characteristics such as dry matter, redox potential, manure pH, exposed manure surface area and manure storage type. These characteristics drive rates of NH_3 volatilization and methanogenesis. In terms of N_2O emissions, T1/2 estimates are driven by N excretion rates, and are calculated by static equations and EF values, which are based on manure management system type (liquid system, solid manure, compost etc.). Conversely, the T3 animal model estimates dairy cow urine and feces as a function of feed composition based on an extant, dynamic, mechanistic model of rumen functioning (Dijkstra et al., 2018). This resulted in T3 N excretion estimates that, as percentage of T1 methodology, ranged from 81 to 98% for the confinement system, depending on the category of cows, to 115–136% for the pasture-based system, depending on each year. The estimates for heifers, in particular, were double those calculated using the T1 approach (211%).

Furthermore, these results indicate that the quality of the feed for cattle impacts the nutrient content and quantity of excretion (Hilgert et al., 2023) in a way that is not captured by the IPCC T1 or 2 approaches. The PB/T3 modelled outputs are considered a more realistic representation of the actual EFs from the farms, and for assessing GHG balances, because they more accurately reflect the impact of input factors known to affect enteric CH_4, N and OM (VS) excretion. In contrast, the T2 approach captures overall N and B_0 and provides a more accurate reflection when conducting generalized comparisons, because it does not require explicit assumptions for each system's important input values. The animal T3 model provides information on excreta N, capturing the effects of dietary changes on enteric CH_4 and excreta composition and volumes. This allows to assess the effects of dietary changes and pasture quality on CH_4 emissions from manure.

Some countries such as Germany and New Zealand have T2 country-specific EFs for many parameters used in calculations of N digestibility, N excretion and N_2O soil emissions. However, for comparisons with IPCC guidelines and not current inventory methodology used by these countries, T1 approach only, is compared with T3 for soil emission category. In addition, T3 results indicated that the mineral soils in these two systems acted as a sink for soil CH_4 which is not presently accounted for in IPCC EFs methodologies.

Direct soil N_2O emissions simulated by the DNDC model were substantially different from T1 estimates in the confinement system and to some extent in the pasture-based systems. Nitrification and denitrification processes are extremely dynamic, both spatially and temporally. These processes are, in turn, intimately related to soil redox potential via water-filled pore space, the timing of field operations, such as grazing and fertilization, which are not included in more empirical/lower Tier approaches (Del Grosso et al., 2015).

4.2. Relevance of process-based models and their limitations

The T3 or PB models require substantially more activity data (climate, soils, fertilizer application time, grazing dates, etc), particularly for the soil emission models and to a lesser extent for the manure storage model. However, they can generate localized case-specific emissions and allow tailored mitigation actions to be more readily measured, reported and verified in specific farm systems. If sufficient activity data and other input data are available, such as specific details on feed type, housing, soils, manure, and climate, the PB models can be useful for comparing individual farm systems and certifying Carbon Farming schemes.

Nevertheless, when the variation in climate and soil conditions is smoothed across farming systems, the advantage of PB models may be lost, and assessment with a T2 approach may be just as suitable. On the other hand, a benefit of the PB models may be to better understand the interaction between a range of mitigation actions. While empirical models are accurate due to their empirical basis, they often lack a representation of underlying processes, for example the effects of feed digestibility and level of DMI on enteric CH_4 emissions. Furthermore, while they may accurately represent emissions under the conditions they are based on, empirical approaches may not perform well when extrapolating beyond the range of conditions they were derived from. In addition, applying empirical equations beyond their range may lead to inaccurate or even unrealistic outcomes. Empirical models in lower Tiers often overlook the influence of digestibility and DMI on CH_4 yield, leading to inadequate representations of variations. Process-based models, as a T3 approach, can account for these factors and provide a comprehensive overview of the variation in estimates of CH_4 emission.

The output from detailed, complex digestion models may contain more detailed data than needed for modelling C and N transformations in manure. However, these models can deliver important characteristics that determine N emission processes after excretion (e.g. urine volume and concentration of ammoniacal N) and during manure storage (e.g. volume of excreta, acidity). The enteric CH_4 outputs were estimated 18–19% higher by the T3 model for the category of high lactating and late lactating, but they were 25% less than the Manure-DNDC model for dry cows. The urine and dung N content have the same tendency. This is because Manure-DNDC model uses empirical equations with feed variables such as NDF and ADF.

Similar to the animal and manure T3/PB models, PB/T3 soil N emissions offer a distinct approach compared to T1 or T2 methods. While T1 and T2 methods rely on a proportion of applied N lost through various pathways (i.e., leaching, volatilization, or nitrification/denitrification), various factors influence PB N emissions such as weather, soil properties, plant N uptake rate, and details in farming management practices (Deng et al., 2015). These factors affect key N transformation processes such as urea hydrolysis, decomposition, nitrification, and denitrification, driving ecosystem N emissions.

PB models show promise in assessing GHG and N emissions at the farm level and predicting the impact of climate change on biogeochemical cycling. They cover diverse farming systems and environmental conditions, offering an advantage over other methods. However, their complexity requires specialized software and limits integration into broader survey tools. Despite limitations, PB models enhance understanding of case-specific farms and monitoring methods, underscoring the importance of transparent documentation for their application as T3 methods (IPCC, 2019a).

4.3. Model evaluation and error analysis

The enteric CH_4 emission predictions from the Dutch T3 model (animal model) for a reference diet had an uncertainty value of 15% for CH_4 EF and 13% for MCF (Bannink et al., 2011). The primary sources of uncertainty in the model's enteric CH_4 emission predictions are errors in feed intake estimation, representation of volatile fatty acid production stoichiometry from the fermented substrate, and rumen pH. Additional uncertainty arises from errors in estimating the dietary and chemical composition of the diets, as well as feed intake (Cf. Table B3; Appendix B). One constraint of utilizing the T3 method is the requirement for more information on the dietary chemical composition and rumen degradation characteristics of feed substrates as inputs. The model was also evaluated well on the prediction of apparent fecal N digestion, which accurately distinguishes between fecal and urinary/ammoniacal N excretion (Bannink et al., 2018).

The DNDC soil model has been thoroughly evaluated against datasets in multiple regions including Germany (Nerger et al., 2020) and New Zealand systems (Giltrap et al., 2015). However, there are uncertainties around model parameters, and modelling assumptions (Giltrap and Ausseil, 2016). In addition, large uncertainties pertain to the measurement data for enteric/manure CH_4 (18%–30%) (Hristov et al., 2018), NH_3 (Bougouin et al., 2016) and soil emissions (Arango and Rice, 2021). Agreement between modelled and measured N_2O emissions has been shown to vary considerably, with R^2 ranging from 0.45 to 0.66 for grazed pastures (Zimmermann et al., 2018) and 0.21 (Macharia et al., 2021) to 0.92 (Deng et al., 2018) for forage cropping systems. The variation in performance was due to uncertainties associated with N_2O emissions and soil properties, particularly SOC, clay content and water filled pore space. In the case of very low R^2 for some cropping systems, this was due to very low observed emissions in very sandy soils with very low nitrification potential. Among the most uncertain parameters in DNDC are those that significantly influence the model outputs such as initial SOC, timing of N application and grazing length. Furthermore, a significant fraction of nitrogen gas (N_2) would be emitted through denitrification, and the N_2 emissions are poorly understood and have not been thoroughly studied (Bracken et al., 2022). In addition, processes, such as the anerobic oxidation of ammonium (NH_4^+) (Ammonox) (Rabbani et al., 2020) are currently not represented in the model, leading to additional uncertainty. However, it is worth noting that the uncertainty is lower in T3 PB modelling compared to T1 and 2 estimates (Deng et al., 2022), presuming that data to constrain the model are available or can be estimated reliably.

Unlike the soil component of DNDC, which has been extensively evaluated for multiple datasets, the housing and storage component of Manure-DNDC has seen limited applications and validation. In this study, the daily and cumulative fluxes of CH_4 and NH_3 in the barn, as estimated by the Manure DNDC model, were evaluated for the first time in the German and European context. This novel application of PB models offers new insights into comprehensive manure management assessments, addressing a significant gap in European-specific research on farm scale GHG and N emissions.

The cumulative observed and modelled values exhibit a higher correlation coefficient ($R^2 = 0.998$ for CH_4 and $R^2 = 0.984$ for NH_3) compared to daily values ($R^2 = 0.07$ for CH_4 and $R^2 = 0.11$ for NH_3). Similarly, the error analysis, as indicated by RMSE and relative RMSE, underlines the models' overall accuracy in capturing cumulative emissions, while daily fluxes show slightly higher relative RMSE, suggesting a proportionally larger deviation in daily predictions. Multiple factors, such as climate and management conditions, affect daily values, leading to significant variability in daily data. Therefore, it can be challenging to establish a good agreement between modelled and observed data, even if the model is accurate. On the other hand, cumulative values integrate the effects of all these factors over a more extended period, thereby reducing the impact of short-term fluctuations and noise. Modelled and observed cumulative values tended to exhibit a higher correlation, making the underlying trends and patterns more apparent.

The bias tests, employing linear regression models, reveal statistically significant p-values for both CH_4 and NH_3 emissions, indicating that the observed and modelled values have a strong correlation. The high R^2 values further support the adequacy of the linear models in explaining the observed-variance relationship.

Studies have reported uncertainty in estimated air exchange of 13% (Ogink et al., 2013) to 49% (Bougouin et al., 2016) due to uncertainties in assumed CO_2 production when using the CO_2 mass-balance approach. Additionally, time-dependent spatial variability of gas dilution within barns, influenced by changing weather conditions and animal activity during fixed sampling setups, introduces further uncertainties (Janke et al., 2020).

The deviation of about 25% between measured and simulated daily emission values in this study is within the range of measurement uncertainty. However, the relative error for NH_3 is considerably higher than that for CH_4. Nevertheless, the recorded daily 65% RMSE remains within reasonable bounds, and several factors contribute to this discrepancy such as the spatial separation of NH_3 and the smaller absolute values of NH_3 compared to CH_4, leading to larger relative errors for NH_3. Therefore, standardized methodologies and PB models could enhance emission estimates and contribute to effective mitigation strategies in dairy systems. For example, optimizing diet formulations can effectively mitigate barn floor emissions, which are highly sensitive to feed rate and CP content (Rodrigues et al., 2022).

5. Conclusions

A novel T3 methodology linking a cascade of PB models across whole farm C and N cycles (animal emissions, housing, manure management, and soil), was compared to results from the IPCC T1 and T2 estimates. This comparison revealed significant differences between PB models and lower IPCC tiers highlighting the need for a more nuanced case-specific approach, where variations in soil type, climate or animal diet may have large impacts on emission estimates. The PB T3 approach captured the interannual variations and accounted for differences in categories of animals, manure management systems and land management. By incorporating localized variations in diet, farm management, soil and climate, it provides a robust framework for accounting and inventory purposes. Consequently, both inventories and C accounting systems can be informed by this PB modelling framework as a potential basis for adopting a more accurate assessment of GHG and N emissions across individual dairy production systems. However, incorporating such a framework into inventories requires addressing challenges related to data availability and quality. Future studies should focus on incorporating comprehensive uncertainty quantification to refine and strengthen the T3 methodology, ultimately improving the accuracy and reliability of GHG inventories. Additionally, PB modelling approaches can also better identify possible trade-offs and synergies between various sources of GHG and N emissions, while capturing interrelationships between farm processes. These approaches are especially pertinent in contexts like 'Carbon Farming,' or domestic offsetting schemes, offering more accurate and nuanced assessments required for subsidies, political regulation, or farm-level applications. Integrating these models into farm assessment tools and carbon foot-printing frameworks would further enhance their practical relevance. Effective strategies for MRV are essential for ensuring data reliability and the success of such initiatives. Finally, the manure-DNDC model effectively simulated cumulative NH_3 and CH_4 barn emissions in the confinement system, reinforcing the value of PB models for assessing GHG emissions. This highlights their potential to advance sustainability efforts within the agricultural sector.

CRediT authorship contribution statement

Latifa Ouatahar: Writing – original draft, Visualization, Investigation, Data curation. **Barbara Amon:** Writing – review & editing, Supervision. **André Bannink:** Writing – review & editing, Validation, Methodology. **Thomas Amon:** Conceptualization. **Jürgen Zentek:** Writing – review & editing. **Jia Deng:** Writing – review & editing, Validation, Methodology. **David Janke:** Writing – review & editing, Validation. **Sabrina Hempel:** Writing – review & editing, Validation, Methodology. **Pierre Beukes:** Writing – review & editing, Validation, Data curation. **Tony van der Weerden:** Writing – review & editing, Validation. **Dominika Krol:** Conceptualization. **Gary J. Lanigan:** Writing – review & editing, Validation, Supervision, Methodology.

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.

Acknowledgments

This article was produced as part of the Capturing Effects of Diet on Emissions from Ruminant Systems (CEDERS) project, a FACCE ERA-GAS-funded project. A. Bannink & G. Lanigan acknowledge EU-Animal Change project and DAFM LABMACC project. The lead author was supported by the TEAGASC Walsh Scholarship Fund and The Leibniz Institute for Agricultural Engineering and Bioeconomy-ATB Potsdam. The participant of J. Deng was supported by California Air Resource Board (contract number: 21RD019). The contribution of Pierre Beukes was supported by New Zealand dairy farmers. The authors thank Detlef May and Kathleen Biscoff for their assistance in data collection. They also acknowledge fruitful discussions with Sebastian Vogel and his assistance with soil data collection.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2024.144479.

Data availability

Data will be made available on request.

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