DEVELOPMENT OF THE CALIFORNIA DAIRY EMISSIONS MODEL (CADEM)

(Contract 19RD028)

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List of Abbreviations

3NOP	3-nitrooxypropanol
ADF	acid detergent fiber (% dry matter)
BW	Body weight
CADEM	California dairy emissions model
CARB	California Air Resources Board
CP	Crude protein (% dry matter)
DMI	Dry matter intake (kg/d)
DNDC	DeNitrification-DeComposition
EE	Ether Extract
EF	Emission Factor
FMPs	Farming management practices
GHG	Greenhouse gases
IPCC	Intergovernmental Panel for Climate Change
NDF	Neutral detergent fiber (% dry matter)
OM	Organic matter (% dry matter)
RRMSE	Relative root mean squared error
R	Coefficient of correlation (%)
USEPA	United States Environmental Protection Agency
VS	Volatile solids
dVS	biodegradable volatile solids
$Water_{in}$	Water intake (kg/d)
MY	milk yield (kg/d)

mPro	milk protein (%)
mFat	milk fat (%)
F_{DM}	fecal DM (kg/d)
F_W	fecal water (kg/d)
F_C	fecal carbon (g/d)
F_N	fecal nitrogen (g/d)
U_t	total urine (kg/d)
U_C	urine carbon (g/d)
U_N	urine nitrogen (g/d)

ABSTRACT

The overall objective of this project is to develop, demonstrate, and transfer to California Air Resources Board (CARB) a comprehensive process-based model, the California dairy emissions model (CADEM), which can be applied to refine estimations of emissions of greenhouse gases (GHG) and nitrogen (N) gases from California dairy farms. Models for enteric fermentation from lactating dairy cattle and heifers were challenged with California-based data and the best performing models were selected. Additionally, manure-related outputs such as fecal and urine amount and composition, and water excretion models were developed. Multivariate models of GHG emissions, manure excretion, and water intake ($Water_{in}$), along with milk production, were developed for lactating cows, nonlactating cows, and heifers. Most equations predicted the response variables with reasonable accuracy, except $Water_{in}$, total urine (U_t), and urine carbon (Uc). No obvious differences were found between multivariate and univariate models because the correlation of random effects between traits was not strong; therefore, the univariate models were selected for CADEM. The emission and excretion models were then integrated with a modified Manure-DNDC. CADEM also simulated the impacts of feed additives on methane (CH_4) emissions from dairy cows. The modifications to Manure-DNDC included incorporation of processes to simulate transfers and interactions of water, carbon (C), N, and phosphorus (P) among multiple slurry storage areas and between slurry storage areas and other components (i.e., housing, digesters, crop fields) within a dairy farm, distinguishing solid and liquid manure during manure transfer. New model interfaces have been developed to improve the usability of CADEM. In addition, the project team has trained CARB staff to gain proficiencies in CADEM and provided materials and guides on applying CADEM.

EXECUTIVE SUMMARY

Background

About 50% of CH_4 emissions in California are attributed to enteric fermentation and manure; therefore, achieving significant CH_4 emission reduction from these sources will be critical to meeting Senate Bill (SB) 1383 goals of reducing methane emissions by 40% by 2030 from 2013 levels. There are different methods for estimating GHG and reactive N gases emissions from dairy farms. For enteric fermentation, the most commonly used methodology worldwide is the Tier 1 or 2 models recommended by Intergovernmental Panel for Climate Change (IPCC, 2006). However, the models do not fully capture the complexity of enteric CH_4 emissions. Although the IPCC (2006) models have been updated recently (IPCC, 2019) based partly on work conducted in California, it is highly recommended to use region-specific models. The Manure-DNDC model was developed to simulate biogeochemical cycles of C, N, and P in livestock farms and can be applied to simulate GHG, ammonia (NH_3), and nitric oxide (NO) emissions from major components of livestock production facilities. However, Manure-DNDC estimates animal CO_2 emissions and C and N excreta primarily based on a prescribed fraction and a mass balance method that may not be able to fully represent impacts of feed ingredients and animal characteristics on GHG emissions and excretion from dairy cattle. Therefore, there is a need to integrate the animal-level and manure-/soil-level dynamics to estimate C and N dynamics in dairy operations with better accuracy than currently available methods. Therefore, the overall objective of this project is to develop, demonstrate, and transfer to CARB a comprehensive process-based model, the California dairy emissions model (CADEM), which can be applied to refine estimations of emissions of GHG and N gases from California dairy farms.

Methods

The project team has developed CADEM by developing prediction equations for enteric CH_4, N and C excretions from cows, and by improving the Manure-DNDC model. Several prediction equations developed over the years were challenged with data from California-based experiments and the best models were selected for inclusion in CADEM. Similarly, prediction equations for urine and fecal outputs including N and C contents were developed and integrated into CADEM. Univariate and multivariate prediction models were compared to determine model performance. Manure-DNDC has been modified to include various processes using mechanistic modeling principles. The results of the animal-based predictions for C and N excretions were used as an input for modified Manure-DNDC.

Results

The improvements made through this project include: 1) integrating Manure-DNDC and UCD fermentation model to predict GHG emissions and manure excretion from dairy cattle, 2) incorporating processes to simulate mitigation of enteric CH_4 emissions due to the use of two types of feed additives (i.e., 3NOP and nitrate), 3) incorporating processes to simulate transfers and interactions of water, C, N, and P among multiple slurry storage areas and between slurry storage areas and other components (i.e., housing, digester, crop fields) within a dairy farm, 4) distinguishing solid and liquid manure during manure transfer, and 5) developing new interfaces to improve the usability of CADEM.

Conclusion

The CADEM simulations of carbon dioxide (CO_2) and CH_4 enteric fermentation emissions, productions of urine C, urine N, and total urine, and productions of fecal C, fecal N, and total fecal from dairy cattle have been evaluated against field observations, and the results indicate that the CADEM can reliably predict these variables. Using the newly developed CADEM, the project team has performed a farm-scale simulation for a real dairy farm in California. The farm-scale simulation demonstrates that the CADEM can be potentially applied to simulate C and N dynamics as well as GHG and NH_3 emissions from major components within a real California dairy farm by equipping model input parameters (e.g., climate, soil, animal, feeding, farm structure, manure storage areas, manure management practices, and farming management practices for crop fields).

Introduction

The agriculture sector represents nearly 60% of California CH_4 emissions, 96% of which comes from enteric fermentation (51%) and manure management (45%) (https://ww2.arb.ca.gov/ghg-inventory-data). California short-lived climate pollutant reduction strategy and SB 1383 have set a CH_4 reduction goal of 40% below 2013 levels by 2030. To achieve this goal, several projects have been conducted to investigate GHG and multiple pollutants emissions from California dairies. The Dairy and Livestock Subgroup #3 organized under SB 1383 generated a document titled, "Dairy Research Prospectus to Achieve California's SB 1383 Climate Goals", which emphasized the need to 1) refine emission inventories using California-specific data in emissions estimation process and 2) evaluate the effectiveness of various mitigation strategies. These recommendations are based on the large variability of California dairy CH_4 emissions due to the wide range of animal and waste management strategies employed in the State. Such variability is not fully reflected in CARB's current emissions inventory due to the lack of California-specific data and a comprehensive modeling platform(s).

In dairy farms, emissions of GHG and N gas (i.e., NH_3, nitrous oxide (N_2O), NO, or dinitrogen (N_2)) can begin soon after feed intake and continue through excretion and all the manure handling processes (Rotz, 2018). The processes involved in GHG and N gas emissions include enteric CH_4 emissions, decomposition of organic manure, methanogenesis, hydrolysis of urea or uric acid, ammonium (NH_4^+) dissociation, NH_3 volatilization, nitrification, and denitrification among other processes (NRC, 2003). A number of factors, such as animal type and age, feed quantity and quality, housing conditions, manure treatment and storage, and manure land application, jointly with the local weather and soil properties, can impact these processes (NRC, 2003; Rotz, 2018). The variability of these controlling factors results in large temporal and spatial heterogeneity of GHG and gaseous N emissions from dairy farms (e.g., Arogo et al., 2006; Owen & Silver, 2015). In addition, the losses of various forms of C and N during one stage of manure treatment may influence the C and N losses during subsequent stages. The intricate transformation of C and N within the manure life cycle has further complicated the quantification and mitigation of GHG and gaseous N emissions at a farm scale (NRC, 2003, Rotz, 2018).

Several models have been developed at University of California, Davis (UCD) (e.g. Moraes et al., 2014; Appuhamy et al., 2016; Niu et al., 2018) to estimate enteric CH_4 emissions. However, the models were not linked to providing inputs for manure CH_4 emission estimation. For estimating manure emissions, the Emission Factor (EF) method has often been utilized for quantifying GHG and N gas emissions at large regional scales (e.g., United States Environmental Protection Agency [USEPA], 2004). EFs are usually generated based on field measurements. However, the measured GHG and reactive N gas emissions data are still scarce and EF approaches based on the measurements are hard to capture the complex combinations of climate, soil, farm types, and manure management practices across different dairy farms. Modeling approaches ranging from statistical regression to processes-based models have been developed to fill the gap. Regression models are developed by relating gas emissions to some determining factors, such as animal type, feed quantity and quality, and climate among others (NRC, 2003). This kind of models may be constrained to the conditions under which the models have been developed (NRC, 2003; Rotz, 2018). In addition, the regression models often lack mechanisms to include some management practices that could potentially reduce GHG and reactive N gas emissions (e.g., Chen et al., 2008; Pinder et al., 2004). In order to improve the quantification and mitigation of GHG and reactive N gas emissions, process-based models have drawn more attention in recent years (e.g., Li et al., 2011; Pinder et al., 2004; Rotz, 2018). Equipped with detailed processes regarding GHG and N gas production and emissions and specifications of farm facilities (Figure 1), these models are able to simulate gas emissions from various farm components (e.g., housing, manure storage, and field with manure application). This results in more refined predictions compared to the use of simple EFs that are commonly applied by the IPCC (Li et al., 2011; NRC, 2003; Rotz, 2018).

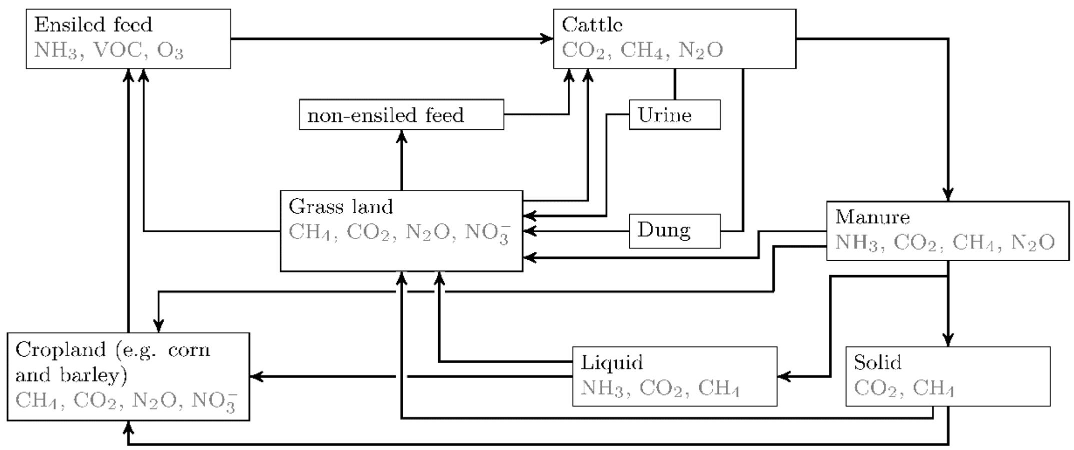

Figure 1. Schematic representation of general framework of the model to be developed and on-farm emission sources.

By considering both natural factors and farming management practices (FMPs) that control C and N dynamics, process-based models have been regarded as useful tools to quantify GHG and N gas emissions, and estimate the mitigation potential of changing FMPs (Butterbach-Bahl et al., 2013; Chen et al., 2008). Manure-DNDC (Li et al., 2012) is an extended version of a process-based soil dynamics model, DNDC (Li et al., 1992a, 1992b; Li, 2000). The latter has been extensively calibrated for California cropping systems and has been used for developing California CH_4 emission inventory from rice paddies and N_2O emission inventory from synthetic fertilizers and crop residue (CARB, 2018; Deng et al., 2018a, b; Figure 2).

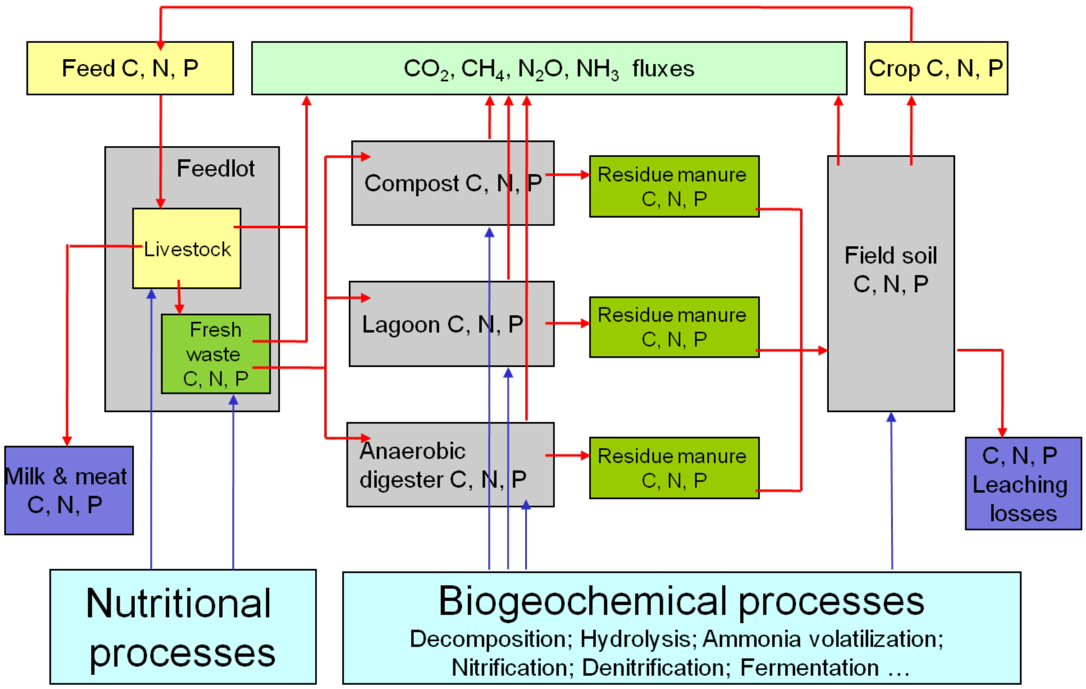

Figure 2. The manure-DNDC framework.

Manure-DNDC contains fundamental processes describing the turnover of manure organic matter (Li et al., 2012). A relatively complete suite of biogeochemical processes, including decomposition, urea hydrolysis, NH_3 volatilization, fermentation, methanogenesis, nitrification, and denitrification, have been embedded in Manure-DNDC, which allows the model to compute the complex transfer and transformations of C, N, and P in livestock production systems. In Manure-DNDC, two bridges have been built to link three basic parts, i.e., farm components (e.g., housing, compost, lagoon, anaerobic digester, and cropping field), environmental factors (e.g., temperature, moisture, air velocity, pH, redox potential, substrates concentration), and biogeochemical processes. The first bridge predicts environmental factors of the farm components based on primary drivers, such as climate, farm structure, characteristics of the facilities, animal type, feed quantity and quality, vegetation, soil properties, and farming management practices. The second bridge links the predicted environmental factors to the biogeochemical reactions (e.g., decomposition, fermentation, methanogenesis, nitrification, and denitrification) that simulate the dynamics of C, N, and P in each farm component. Losses of C, N, and P through gas emission, runoff, or leaching are calculated as part of the biogeochemical cycles of the three elements across the livestock farm components (Figure 2) (Li et al., 2012). The model has been used to estimate GHG and NH_3 emissions from isolated dairy facilities in several states (Deng et al., 2015; Li et al., 2012).

Manure-DNDC has not been well parameterized for California dairies and does not incorporate all of the California dairy components that are sources of GHG and N gas emissions (e.g., solid-liquid separation including settling basins). In addition, Manure-DNDC estimates animal CO_2 emissions and amount of C and N excreta primarily based on a prescribed fraction and a mass balance method (Li et al., 2012) that may not be able to fully represent impacts of feed ingredients and animal characteristics on GHG emissions and excretion from dairy cattle. To fill these gaps, this project has focused on development of CADEM. The overall objective of this project is to develop, demonstrate, and transfer to CARB a comprehensive process-based California dairy emissions model that can be applied to refine estimations of emissions of GHG and N gas from California dairy farms. The following specific objectives were addressed in the current study:

1. Compile data and review emissions of CH_4, NH_3, N_2O, CO_2, NO, and N_2 from California dairies
2. Develop CADEM based on the Manure-DNDC and UCD enteric fermentation model to simulate GHG and N gas emissions.
3. Expand CADEM to include simulations of CH_4, NH_3, N_2O, CO_2, NO, and N_2 emissions from all dairy components.
4. Calibrate, validate, and improve the CADEM

5. Apply CADEM to estimate efficiencies of alternative dairy practices in mitigating CH_4, NH_3, N_2O, CO_2, NO, and N_2 emissions from California dairies
6. Produce an easy-to-use graphical user interface (GUI) of CADEM and train CARB staff

Diet Database Construction

A database that contains the composition of diets commonly fed at California dairy farms is required for an accurate prediction of GHG emissions from dairy cattle. Such a database was collated from dairy experiments performed in California that were published recently, that is from 2010 onwards. Before including studies in the database, dietary treatments were screened and data from treatments using specific supplements that are not described by common macro- and micro-nutrients were not included, which often resulted in the control treatment only. The database comprised 66 treatments from the following 13 studies: Cassinerio et al., 2015; Havlin et al., 2015; Naranjo et al., 2020; Niu et al., 2016; Rauch et al., 2012; Robinson et al., 2010; Robinson et al., 2011; Robinson et al., 2012; Roque et al., 2019; Swanepoel et al., 2010; Swanepoel et al., 2014; Swanepoel et al., 2018; Tewoldebrhan et al., 2017. Treatments that included supplements that are not easily described by commonly used dietary nutrients were removed from the dataset, which applied to: Robinson et al. (2010; 1 rumen protected lysine and 1 rumen protected amino acids product), Robinson et al. (2011; 1 rumen protected lysine treatment), Cassinerio et al. (2015; 3 tomato seed treatments), Tewoldebrhan et al. (2017; 2 β-mannanase treatments), Swanepoel et al. (2018; 3 treatments with rumen protected methionine, phenylalanine and tyrosine) and Roque et al. (2019; 2 β-mannanase treatments). 53 dietary observations were retained after the removal of these treatments, after which dietary nutrient content of neutral detergent fiber (NDF), acid detergent fiber (ADF), lignin, crude protein (CP), fat, ash, and P were calculated from dietary ingredient composition using Table values of the NRC (2001). Furthermore, samples were drawn from uniform distributions for body weight (BW), days in milk, and milk protein percentage. Boundaries for the uniform distribution were 600 and 800 kg BW for Holstein cows and 450 and 550 kg BW for Jersey cows, 0 and 305 days in milk with dry cows assigned 365 days in milk, 2.45% and 4.09% for milk protein percentage. Kernel densities, i.e. a non-parametric way to estimate the probability density function of a random variable, were then estimated per dietary and animal variable and are shown in Figure 3. These identify whether a certain variable is normally distributed or has skewed distribution that many necessitate further description. Most of the diet characteristics are normally distributed so it can be described by the averages.

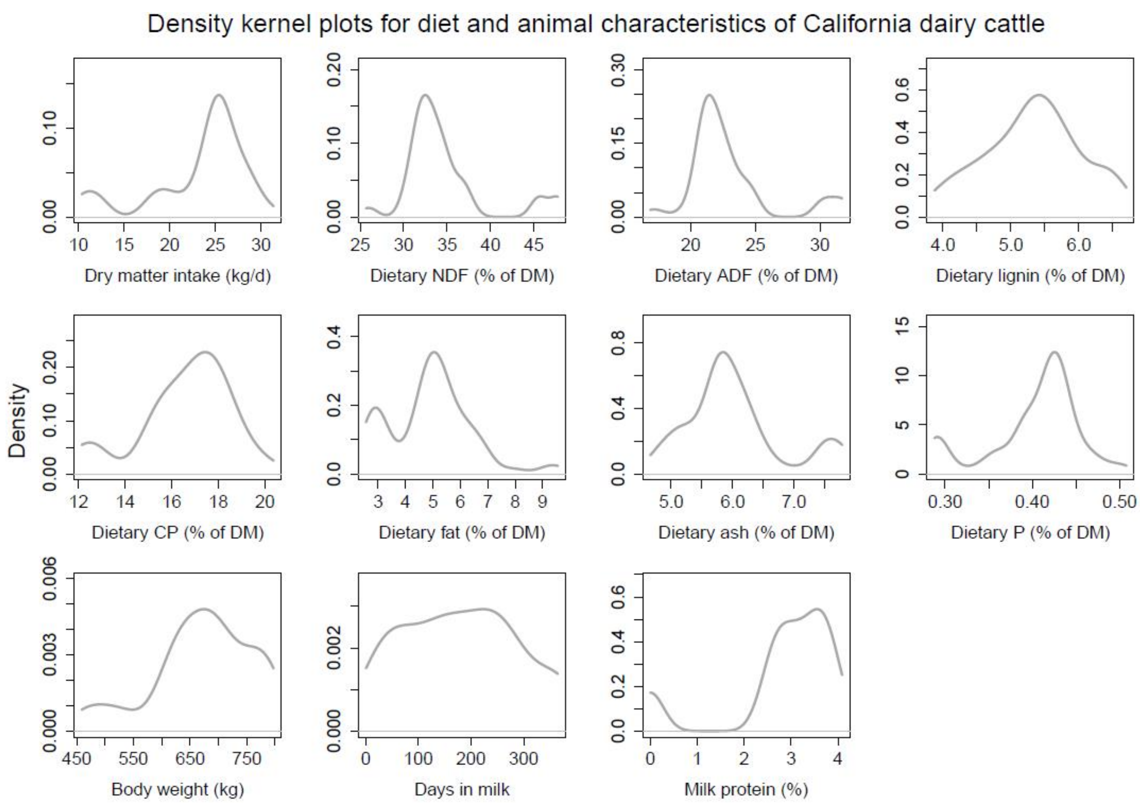

Figure 3. Density kernel plots for diet and animal characteristics of California dairy cattle.

Development of Enteric Fermentation Model

Lactating dairy cows

Many equations have been developed to predict CH_4 emissions from dairy cattle. Appuhamy et al. (2016) evaluated 40 CH_4 emission predicting equations developed in North America, Europe, Australia, and New Zealand. Niu et al. (2018) built eleven equations to predict CH_4 emissions. In order to find an appropriate equation, which can well represent CH_4 emission by dairy cattle in California, data from three experiments (Niu et al., 2016; Tewoldebrhan et al., 2017; Roque et al., 2019) conducted in California were used to evaluate the predictability of four equations, two of which were selected from Appuhamy et al. (2016):

$$CH_4 = (1.23\ DMI - 1.45\ FA + 0.120\ NDF)/0.05565 \qquad (1)$$

$$CH_4 = exp\ (3.15 - 0.035\ EE)\ DMI \qquad (2)$$

The other two were selected from Niu et al. (2018):

$$CH_4 = 49.5 + 2.57\ NDF + 12.1\ DMI \qquad (3)$$

$$CH_4 = 136 + 12.3\ DMI - 2.96\ EE \qquad (4)$$

where CH_4 = Daily methane emissions (g/d), DMI = Dry matter intake (kg/d), FA = Dietary fatty acid content (% of DM), NDF = Dietary NDF content (% of DM), EE = Dietary fat content (% of DM).

All the equations were selected based on the rank in the studies and the availability of the covariates. The three datasets contained 254 observations in total. None of the datasets provided the information on FA, thus the following equation developed by Palmquist et al. (2003) was used to estimate dietary FA content:

$$FA = -0.98 + 1.03\ EE \tag{5}$$

Root mean squared error of prediction (RMSEP) and concordance correlation coefficient (CCC; Lawrence and Lin, 1989) were used to evaluate the accuracy and precision of the four equations.

Table 1. Root mean square error of prediction (RMSEP) and concordance correlation coefficient (CCC) of four equations.

Equation	RMSEP, % of mean observed value	CCC
(1)	43.01	0.21
(2)	37.99	0.23
(3)	26.71	0.27
(4)	26.77	0.28

As shown in Table 1, equations 3 and 4 were very close and out-performed equations 1 and 2. The equation 3 was selected for use to estimate CH_4 emissions in CADEM.

Through this project, we have integrated the UCD enteric model into CADEM to predict GHG emissions and manure excretion (i.e., volatile solid in manure, water, C, and N in urine and fecal parts of manure) from dairy cattle. Specifically, a group of the empirical equations developed by the UCD group (Table 2) has been seamlessly integrated into the code of the CADEM model. These equations can be used to simulate dairy CO_2 emission, enteric CH_4 emission, and dairy excretion (e.g., water, C, and N amounts in manure) from California dairy cattle. The predicted CO_2 and CH_4 emissions, as well as dairy excretion would be reported on a daily basis. The dairy excretion goes through other processes in manure life cycle (e.g., transfers from housing to manure storage areas and/or lands receiving manure, manure transformation through physical, chemical, or biogeochemical processes). GHG emissions from manure storage areas and/or lands can be simulated by CADEM as well by tracking manure transfers and transformation.

Table 2. Equations for calculating dairy CO2 emission, enteric CH4 emission, and dairy excretion. The equations were from the UCD fermentation model.

Equations		Notes
[6]	CO_2 flux = 0.55×DMI	Daily CO_2 flux
[7]	CH_4 flux = 49.5+12.1×DMI+2.57×NDF	Daily enteric CH_4 flux
[8]	Urine = -7.742+0.388×DMI+0.726×CP+2.066×MPR	Daily urine amount
[9]	UrineC = -0.1601 +0.0082×DMI+0.0107×CP+0.00013×BW	Daily urinary C excretion
[10]	UrineN = -166+5.75×DMI+13.1×CP	Daily urinary N excretion
[11]	Fecal water = 1.987×DMI+0.348×ADF-0.412×CP-0.074×DM-0.0057×DIM	Daily fecal water amount
[12]	FecalC = 0.169×DMI-0.034×CP+0.027×ADF-0.075×MPR	Daily fecal organic C excretion
[13]	FecalN = -58.3+9.07×DMI+0.902×ADF+2.14×CP	Daily fecal organic N excretion
[14]	Volatile solids = -1.201+0.402×OMI+0.036×NDF-0.024×CP	Daily volatile solids excretion
Definitions of variables listed in equations		

ADF	Acid detergent fiber content in feed
BW	Cow body weight
CP	Crude protein content in feed
DIM	Days in milk
DM	Dry matter content in fresh feed
DMI	Daily dry matter intake rate
MPR	Milk protein percentage
NDF	Neutral detergent fiber content in feed
OMI	Organic matter intake

The applications of the UCD fermentation model require new model input parameters of feed ingredients (e.g., organic matter (OM), fat, ADF, NDF, and lignin contents in feed; see Table 2). To facilitate the applications, the Manure-DNDC database of feed ingredients information has been expanded and updated to form the CADEM database by including the new required information. Currently, around 120 feed types with ingredients information have been included in the database (see Table 3 for the database example). In addition, we have created new model interfaces (Figures A1 and A2) to receive new input parameters (i.e., dry matter faction in feed, milk protein content, cow body weight, and days in milk), to calculate input parameters of feed ingredients based on feed types, and to allow model users to choose different options, the UCD fermentation model or the original functions in Manure-DNDC, for simulating dairy CO_2 flux, enteric CH_4 flux, and dairy excretion. These new interfaces provide flexibility in preparing model inputs because they allow users to estimate feed ingredient parameters based on feed types. They also facilitate conducting simulations of dairy CO_2 flux, enteric CH_4 flux, and dairy excretion based on data availability.

Table 3. Example of updated feed ingredients (in percentage) information.

ID	Feed type	DM	CP	FAT	NDF	ADF	Lignin	Ash	P
1	Alfalfa	90.3	19.2	2.5	41.6	32.8	7.6	11	0.28
2	Almond	86.9	6.5	2.9	36.8	28.7	14.9	6.1	0.13
3	Apple	35.9	7.7	5	52.5	43.2	15.4	2.6	0.14
4	Bakery byproduct	84.7	12.5	9.5	13.9	6.5	1.6	3.8	0.36
5	Barley (grain)	91	12.4	2.2	20.8	7.2	1.9	2.9	0.39
6	Barley (spouts)	90.5	20.1	2.3	47	21.8	3.4	7.4	0.51
7	Barley (silage)	35.5	12	3.5	56.3	34.5	5.6	7.5	0.3
8	Beet (sugar)	88.3	10	1.1	45.8	23.1	1.6	7.3	0.09
9	Bemudagrass	87.1	10.4	2.7	73.3	36.8	6.5	8.1	0.27
10	Blood	90.2	95.5	1.2	NA	NA	NA	2.5	0.3
11	Brewers (grain)	90.7	29.2	5.2	47.4	22.2	5	4.3	0.67
12	Canola (seed)	89.9	20.5	40.5	17.8	11.6	2.7	4.6	0.68
13	Chocolate	95.2	11.9	20.5	23.8	15.7	3.2	2.1	0.3
14	Citrus	85.8	6.9	4.9	24.2	22.2	0.9	7.2	0.12
15	Corn (cobs)	90.8	3	0.6	86.2	42.2	5.9	2.2	0.06
16	Corn (distillers grain)	90.2	29.7	10	38.8	19.7	4.3	5.2	0.83
17	Corn (gluten feed)	89.4	23.8	3.5	35.5	12.1	2	6.8	1
18	Corn (gluten meal)	86.4	65	2.5	11.1	8.2	1.5	3.3	0.6
19	Corn (grain cracked)	88.1	9.4	4.2	9.5	3.4	0.9	1.5	0.3
20	Corn (grain ground dry)	88.1	9.4	4.2	9.5	3.4	0.9	1.5	0.3
21	Corn (grain steam flaked)	88.1	9.4	4.2	9.5	3.4	0.9	1.5	0.3
22	Corn (grain rolled)	71.8	9.2	4.3	10.3	3.6	0.9	1.5	0.3

The CADEM interface has also been updated to allow model users to set feed additive input parameters, including type and amount, to apply the function of simulating impacts of feed additive on enteric CH_4 emissions (please refer to the section of "Develop CADEM to simulate effects of feed additives on mitigating CH_4 flux from cattle"). The new added processes and updated interface would enable CADEM to simulate the CH_4 reduction potential of 3NOP and nitrate for both beef and dairy cattle. As more studies on impacts of feed additives on mitigating enteric CH_4 flux is conducted, we expect that these equations would be updated and more types of feed additives would be included in CADEM.

Heifers

Enteric CH_4 emissions from heifers may not be the same as lactating dairy cattle. Therefore, we evaluated 18 mathematical models developed by Moraes et al. (2014), Jiao et al. (2014), US EPA (dairy heifers), IPCC (2019), Van Lingen et al. (2018), and Charmley et al. (2016). Table 4 shows the summary of the data (from experiments conducted over 40 years at the USDA Energy Metabolism unit (Bethesda, MD)) used for evaluation of heifer's CH_4 prediction equations and Table 5 shows model performance on predicting CH_4 emission for heifers for the 18 equations:

Table 4. Summary of data (n=458) used for evaluation of heifer's CH_4 prediction equations

Variable	Mean	SD	Minimum	Maximum
Gross energy intake, MJ/d	100	27.37	47.37	185
DMI, kg/d	5.12	1.36	2.56	9.78
Ether extract (EE), %	3.51	1.46	0.67	7.55
NDF, %	42.38	15.12	17.88	78.29

Forage, %	91.88	17.96	35.31	100
CH_4 emission, g/d	114	32.62	46.63	230

Table 5. Model performance on predicting CH_4 emission for heifers of 18 equations (n = 458)

Eq. No.	Equation	RMSPE, % of mean	RSR	ccc	Mean bias, % of MSPE	Slope bias,% of MSPE
15	Moraes et al. 2014 H	15.24	0.53	0.82	0.61	2.45
16	Moraes et al. 2014 H	18.74	0.65	0.77	3.88	3.58
17	Moraes et al. 2014 NL	26.35	0.92	0.62	67.25	0.33
18	Moraes et al. 2014 NL	24.06	0.84	0.66	62.19	0.69
19	Jiao et al. 2014	17.33	0.60	0.81	21.62	1.45
20	US EPA (dairy heifers)	16.40	0.57	0.82	15.81	0.43
21	IPCC 2019	15.27	0.53	0.85	0.01	3.37
22	Van Lingen et al. 2019 [12]	19.17	0.67	0.69	20.45	16.68
23	Van Lingen et al. 2019 [13]	23.22	0.81	0.62	32.66	0.19
24	Van Lingen et al. 2019 [14]	20.96	0.73	0.80	96.62	0.44
25	Van Lingen et al. 2019 [15]	19.58	0.68	0.67	12.75	10.02
26	Van Lingen et al. 2019 [16]	33.52	1.17	0.37	61.45	0.60
27	Van Lingen et al. 2019 [38]	17.09	0.60	0.75	5.23	15.62
28	Van Lingen et al. 2019 [39]	20.66	0.72	0.69	4.85	1.31
29	Van Lingen et al. 2019 [40]	27.82	0.97	0.71	45.89	0.09

30	Van Lingen et al. 2019 [41]	18.86	0.66	0.70	12.89	6.37
31	Van Lingen et al. 2019 [42]	29.83	1.04	0.44	50.46	0.12
32	Charmley et al. 2016	16.13	0.56	0.82	10.99	0.23

The best models for predicting emission from heifers were IPCC (2019), Moraes et al. (2014), Van Lingen et al. (2019 model 38) and Charmely et al. (2016). Given that the IPCC (2019) is an internationally recognized standard (also developed with some California data) and easy to implement, we recommend the following IPCC (2019) to be used to estimate CH_4 emissions from dairy heifers.

$$CH_4\ (MJ/d) = 0.063 \times Gross\ energy\ intake\ (MJ/d) \quad (33)$$

Multivariate and Univariate Models to Predict Greenhouse Gas Emission, Manure Excretion and Water Intake in Dairy Cattle

Several studies have investigated the mitigation strategies (e.g., Waghorn et al., 2008; Klop et al., 2016; Honan et al., 2021), measurements (e.g., Pinares-Patiño et al., 2008; Hammond et al., 2016), and prediction (e.g., Moraes et al., 2014; Appuhamy et al., 2016a; Niu et al., 2018) of enteric CH_4 emissions for dairy cattle. Manure produced by animals generates CH_4, N_2O and NH_3 through decomposition, hydrolysis, nitrification and denitrification processes (Li et al., 2012). The organic matter (or volatile solids, VS) in manure is closely related to the potential CH_4 production from manure and is used as a predictor for CH_4 production in the Intergovernmental Panel on Climate Change (IPCC) Tier 2 methodology (IPCC, 2006). However, lignin in manure is resistant to anaerobic digestion and does not contribute to CH_4 production, therefore VS without lignin, also known as biodegradable VS (dVS) is a better predictor for manure CH_4 (Appuhamy et al., 2018). Various prediction models dealing with whole farm emissions, including emissions at animal, manure and soil levels have been developed in recent years (e.g., Li et al., 2012; Rotz et al., 2014). The quantification of detailed manure compositions, including carbon, nitrogen and water content, can provide inputs for these whole-farm models. Water intake ($Water_{in}$) is essential to milk production, and to predicting manure water excretion and overall water footprint at animal level.

Most extant models for the prediction of GHG emissions, manure excretion and $Water_{in}$ are univariate (e.g., Appuhamy et al., 2014; Niu et al., 2018). However, univariate models do not take correlations between response variables into consideration and may lead to model bias (Moraes et al., 2015). Van Lingen et al. (2018) developed a multivariate model to predict emissions and excretion for dairy cows, but the model only includes CH_4, dVS and manure nitrogen as the response variables. In this study, we aimed to develop a multivariate model to predict CH_4, CO_2, VS, dVS, manure carbon and nitrogen, water intake for dairy cattle and compare them with univariate model to determine which equations should be used in CADEM. Most studies focus on the environmental effects of lactating cows alone, therefore, we expanded the model to include nonlactating cows and heifers to enable the assessment of environmental impact at the whole farm level.

Data sources

A dataset containing individual records of CH_4 production, manure excretion and water intake from Holstein and Jersey lactating (n = 1111) and nonlactating (n = 591) cows, and Holstein, Jersey and Angus-Hereford cross heifers (n = 414) was assembled. Records were collected in 53 trials at the former USDA Energy Metabolism Unit at Beltsville, Maryland from 1963 to 1995. Descriptive statistics for the variables used in this study are shown in Table 6.

Table 6. Descriptive statistics of diet compositions, animal status emission and excretion for the dataset used in this study

Item*	Lactating cows (n = 1111)			Nonlactating cows (n = 591)			Heifers (n = 414)		
	Mean (SD)	Min	Max	Mean (SD)	Min	Max	Mean (SD)	Min	Max
CP, % of DM	16.2 (2.5)	5.2	23.5	16.0 (2.4)	4.9	21.8	15.6 (2.9)	10.4	23.6
NDF, % of DM	34.3 (7.5)	14.9	76.1	36.3 (10.0)	14.0	74.0	41.2 (14.9)	13.2	78.3
ADF, % of DM	20.0 (4.2)	7.7	47.1	21.6 (6.9)	5.0	47.4	24.6 (11.4)	4.3	48.3
Lignin, % of DM	4.4 (1.4)	0.5	9.4	4.8 (2.0)	0.8	14.3	5.2 (2.7)	0.4	13.5
EE, % of DM	2.8 (1.0)	1.0	7.0	2.7 (0.9)	0.8	7.6	2.9 (1.1)	0.9	6.3
Ash, % of DM	6.4 (1.1)	3.7	12.1	7.3 (2.3)	3.5	22.1	6.4 (1.9)	3.1	13.7

DM, % of diet	65.3 (19.8)	30.2	97.4	67.9 (20.9)	19.4	98.7	56.2 (27.0)	19.7	97.0
DMI, kg	16.5 (4.3)	3.9	29.4	6.7 (2.0)	2.3	13.4	5.4 (1.6)	1.8	12.8
OMI, kg	15.4 (4.0)	3.6	27.3	6.2 (1.9)	2.1	12.8	5.0 (1.5)	1.7	11.9
DIM, d	162 (82.1)	11.0	488	-	-	-	-	-	-
BW, kg	594 (88.6)	302	854	668 (88.4)	328	893	345 (72.9)	195	542.0
MY, kg/d	23.3 (10.3)	0.1	56.6	-	-	-	-	-	-
mPro, %	3.3 (0.4)	2.3	5.8	-	-	-	-	-	-
mFat, %	3.67 (0.75)	1.42	7.6	-	-	-	-	-	-
CH_4, g/d	298 (91.8)	68.3	551	162 (43.1)	42.4	322.9	119 (37.6)	47.9	248
CO_2, kg/d	10.6 (2.1)	3.7	17.1	6.4 (1.3)	2.2	10.3	4.6 (1.1)	2.4	8.5
$Water_{in}$, kg/d	60.5 (28.3)	2.0	121.3	24.6 (14.9)	1.0	124.4	14.3 (10.8)	0.2	109.2
VS, kg/d	5.9 (1.8)	1.5	12.1	2.2 (0.9)	0.7	6.1	1.9 (0.7)	0.4	7.8
dVS, kg/d	5.3 (1.6)	1.4	11.4	2.0 (0.8)	0.7	5.8	1.7 (0.6)	0.4	7.6
F_{DM}, kg/d	5.5 (1.8)	1.1	11.2	1.9 (0.8)	0.5	5.5	1.7 (0.6)	0.3	4.1
F_W, kg/d	27.1 (10.2)	4.8	65.9	8.1 (4.1)	1.5	29.7	6.6 (3.0)	1.0	21.6
F_C, g/d	2541 (798.2)	539	5208	882 (383.9)	215	2626	789 (302.2)	143	2017
F_N, g/d	150 (54.8)	35.1	377.6	51.2 (19.1)	13.2	125.2	46.9 (18.3)	11.8	119.4
U_t, kg/d	17.5 (8.9)	4.4	138.3	15.9 (11.4)	2.5	103.8	9.6 (5.0)	1.8	31.8
U_C, g/d	232 (99.9)	12.1	1925	137 (71.0)	29.2	1115	99.5 (78.7)	29.4	237.4
U_N, g/d	152 (65.8)	22.3	363	108 (37.1)	17.0	248	71.7 (34.2)	18.1	212.5

* MY = milk yield, mPro = milk protein, mFat = milk fat, VS = volatile solids, dVS = biodegradable volatile solids, F_{DM} = fecal DM, F_W = fecal water, F_C = fecal carbon, F_N = fecal nitrogen, U_t = total urine, U_C = urine carbon, U_N = urine nitrogen

Multivariate Model

A total of 12 variables, including CH_4 (g/d), CO_2 (kg/d), water intake (kg/d), VS (kg/d), dVS (kg/d), fecal DM (F_{DM}, kg/d), fecal water (F_W, kg/d), fecal carbon (F_C, g/d), fecal nitrogen (F_N, g/d), total urine (U_t, kg/d), urine carbon (U_C, g/d) and urine nitrogen (U_N, g/d), were predicted by a multivariate model for lactating cows, nonlactating cows and heifers. However, VS and dVS were not available directly in the dataset. Urine organic matter (OM) is approximately 4 times of urine carbon (Dijkstra et al. 2013), therefore, VS was calculated as the sum of measured fecal OM and 4 times the measured U_C, i.e., VS = fecal OM + 4 U_C (Appuhamy et al., 2018). Then dVS was obtained by subtracting fecal lignin from VS.

A Bayesian multivariate model was constructed as follows:

$$\mathbf{Y} = \mathbf{X}\,\mathbf{B} + \mathbf{Z_1}\,\mathbf{\Delta} + \mathbf{Z_2}\,\mathbf{A} + \mathbf{E} \quad [i]$$

where $\mathbf{Y}$ is an n × r matrix, with each row representing r (r = 12) response variables or columns of each observation; $\mathbf{X}$ (n × m), $\mathbf{Z_1}$ (n × j) and $\mathbf{Z_2}$ (n × k) are the design matrices relating $\mathbf{B}$, $\mathbf{\Delta}$ and $\mathbf{A}$ to $\mathbf{Y}$; $\mathbf{B}$ is an m × r matrix with each row representing the regression coefficients predicting each response variable; $\mathbf{\Delta}$ is a j × r matrix with each row representing the study random effects on each response variable; $\mathbf{A}$ is k × r matrix with each row representing the animal random effects on each response variable; $\mathbf{E}$ is an n × r error matrix; n, j, k, and m represent the number of observations, studies, animals, and covariates, respectively. Animal was included as a random effect because one animal was used in multiple studies and had multiple observations. To understand the distributions of error, study and animal random effect, consider $\mathbf{\Delta}$, $\mathbf{A}$ and $\mathbf{E}$ matrices as stacked column-wise $\boldsymbol{\delta}$, $\boldsymbol{\alpha}$ and $\boldsymbol{\epsilon}$ vectors:

$$\mathbf{\Delta} = [\boldsymbol{\delta}_1\ \boldsymbol{\delta}_2 \ldots \boldsymbol{\delta}_r],\ \mathbf{A} = [\boldsymbol{\alpha}_1\ \boldsymbol{\alpha}_2 \ldots \boldsymbol{\alpha}_r],\ \mathbf{E} = [\boldsymbol{\varepsilon}_1\ \boldsymbol{\varepsilon}_2 \ldots \boldsymbol{\varepsilon}_r]$$

$$\boldsymbol{\delta} = \begin{bmatrix} \boldsymbol{\delta}_1 \\ \boldsymbol{\delta}_2 \\ \vdots \\ \boldsymbol{\delta}_r \end{bmatrix}, \boldsymbol{\alpha} = \begin{bmatrix} \boldsymbol{\alpha}_1 \\ \boldsymbol{\alpha}_2 \\ \vdots \\ \boldsymbol{\alpha}_r \end{bmatrix}, \boldsymbol{\epsilon} = \begin{bmatrix} \boldsymbol{\epsilon}_1 \\ \boldsymbol{\epsilon}_2 \\ \vdots \\ \boldsymbol{\epsilon}_r \end{bmatrix}$$ [ii]

where $\boldsymbol{\delta}_p$, $\boldsymbol{\alpha}_p$ and $\boldsymbol{\epsilon}_p$ are the study random effect, animal random effect and error vectors, respectively for p = 1 to r. Then the distribution of $\boldsymbol{\delta}$, $\boldsymbol{\alpha}$ and $\boldsymbol{\epsilon}$ was:

$$\begin{bmatrix} \boldsymbol{\delta} \\ \boldsymbol{\alpha} \\ \boldsymbol{\epsilon} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{I_j} \otimes \mathbf{G}_{\boldsymbol{\delta}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I_k} \otimes \mathbf{G}_{\boldsymbol{\alpha}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I_n} \otimes \mathbf{R}_{\boldsymbol{\epsilon}} \end{bmatrix} \right)$$ [iii]

where $\mathbf{I_j}$, $\mathbf{I_k}$ and $\mathbf{I_n}$ are identity matrices of order j, k and n, respectively; $\mathbf{G}_{\boldsymbol{\delta}}$, $\mathbf{G}_{\boldsymbol{\alpha}}$ and $\mathbf{R}_{\boldsymbol{\epsilon}}$ are unstructured covariance matrices of order r for $\boldsymbol{\delta}$, $\boldsymbol{\alpha}$ and $\boldsymbol{\epsilon}$, respectively. Minimally informative distributions were specified for the priors so that the inference is mostly influenced by the observed data (Gelman et al., 2004). All the regression coefficients were set to follow a normal prior with 0 mean and variance equal to 10^{10}. Inverse Wishart priors were specified for covariance matrices with degrees of freedom equal to 0.1 and scale matrix equal to $10^4\,\mathbf{I_r}$, where $\mathbf{I_r}$ is an identity matrix of order r.

Covariates for model selection included breed, DMI, OM intake (OMI), days in milk (DIM), BW, age, milk yield (MY), milk protein (mPro), milk fat (mFat), and dietary contents of NDF, ADF, CP, EE, lignin and ash. Model selection was based on deviance information criterion (DIC). A decrease of DIC value by more than 10 units indicates a substantial improvement by an additional covariate (Spiegelhalter et al., 2002). Otherwise, the covariate was considered unnecessary. Given the multivariate model contained 12 response variables and 15 covariates, the computation load of a greedy search for the best model was extremely heavy. Instead, a bidirectional selection was conducted in this study (Draper and Smith, 1998). At each step, all possible additions and deletions of a single covariate were made, and the action that improves

DIC the most was taken. The procedure was repeated until no improvement can be made, or the improvement of DIC was less than 10 units, for each of the response variable one by one.

The Markov Chain Monte Carlo (MCMC) was generated using Gibbs sampling. After checking the MCMC convergence based on graphical methods, including trace, autocorrelation and running mean plots (Roy, 2020), the chain length was set to be 1.1×10^5 with the first 10^4 iterations removed as burn-in and chain thinning of 25. All the models were developed using the MCMCglmm package (Hadfield, 2010) in R (version 4.1.2, R Foundation for Statistical Computing, Vienna, Austria).

Univariate Models

To compare performance of multivariate vs. univariate models given our dataset, all regression coefficients were estimated using a univariate Bayesian regression model based on similar procedures described above, except the multivariate structure was switched to a univariate one. The statistic model is as follows:

$$y_{ip} = \beta_0 + \beta_1 x_{ip1} + \beta_2 x_{ip2} + \cdots + \beta_s x_{ips} + \delta_s + \alpha_a + e_{ip} \qquad \text{[iv]}$$

where y_{ip} is response variable p from observation i; β_0 is the slope; x_{ip1} to x_{ips} are covariates related to slopes β_1 to β_s; δ_s and α_a are the study and animal random effects related to observation i; e_{ip} is the random error. The study, animal, and error terms are distributed as $\delta_s \sim N(0, \sigma_\delta^2)$, $\alpha_a \sim N(0, \sigma_\alpha^2)$, and $e_{ip} \sim N(0, \sigma_e^2)$, respectively. Similar to multivariate models, all the regression coefficients were set to follow a normal prior with 0 mean and variance equal to 10^{10}. Inverse Wishart priors were specified for study, animal and error variances with degrees of freedom equal to 0.1 and scale parameter equal to 10^4.

All the covariates in the univariate models were kept the same as those in multivariate models without selection, so that we could examine whether multivariate models predict the response variables better than univariate ones given the same set of covariates.

Model Evaluation

All the multivariate and univariate models for three animal groups were evaluated using the K-fold cross-validation method (Efron and Tibshirani, 1993), in which folds were individual studies (K = number of studies). Each fold was used as a validation set, and its predicted response variables were calculated based on the model fitted from the remaining folds. The goodness of model prediction was assessed by the root mean square prediction error (RMSPE; Bibby and Toutenburg, 1977), RMSPE to standard deviation of observed values ratio (RSR; Moriasi et al., 2007), mean bias (MB), and slope bias (SB).

An independent test dataset containing CH_4 emissions for lactating cows was used to examine the prediction accuracy of the CH_4 emission equation developed in this study. The independent dataset was collected from the three trials conducted in the US, and included 161 observations, 48 of which were from Niu et al. (2016), 36 of which were from Tewoldebrhan et al. (2017), and 77 from Roque et al. (2019). The prediction accuracy of the equations developed in the current study was compared with three published equations (Table 7). Only the CH_4 emission equation for lactating cows was examined due to the lack of independent data for the other variables.

Table 7. Methane prediction equations used for the comparison with our equation for lactating cows

Eq.	Reference	Prediction equation*
34	Niu et al., 2018	$-126 + 11.3 \times \text{DMI} + 2.30 \times \text{NDF} + 28.8 \times \text{mFat} + 0.148 \times \text{BW}$

35	Moate et al., 2011	$e^{(3.15 - 0.035 \times EE)} \times DMI$
36	Moraes et al., 2014	$-9.311 + 0.042 \times GEI + 0.094 \times NDF - 0.381 \times EE + 0.008 \times BW + 1.621 \times mFat$

* mFat = milk fat (% of milk), GEI = gross energy intake (MJ/d)

The final selected multivariate models for lactating cows, nonlactating cows and heifers are shown in Table 8,

Table 9, and Table 10, respectively. All the equations contained an intercept for lactating and nonlactating cows, but all the equations for heifers did not except F_W, F_C, and F_N. The intercepts were excluded from those equations because they were highly varied (SD > 10 × mean), which could cause a model bias and undermine the cross validation. The most important factor of predicting GHG emissions and manure excretions was feed intake (DMI or OMI), which was contained in all the equations except the U_t equation for nonlactating cows. Compared to DMI, OMI excludes ash and should be theoretically more relevant to GHG emissions and manure OM excretions (Appuhamy et al., 2018). Although several equations contained OMI instead of DMI based on the model selection, we only found minor differences on the results of DIC and cross validation between models replacing DMI with OMI or vice versa, because of the small difference between DMI and OMI. Breed was not present in any equations in the final selected models. Similarly, Moraes et al. (2014) did not find any significant effects of breed on emissions when dietary compositions and animal status were considered, indicating a similar biological process of producing GHG production and manure excretions shared by bovine breeds (Klevenhusen et al., 2011).

Table 8. Selected multivariate model and root mean square prediction error (RMSPE, % of observed mean) for enteric CH_4 (g/d), CO_2 (kg/d), water intake ($Water_{in}$, kg/d), milk yield (MY, kg/d), fecal DM (F_{DM}, kg/d), fecal nitrogen (F_N, g/d), fecal carbon (F_C, g/d), fecal water (F_w,

kg/d), total urine (U_t, kg/d), urine nitrogen (U_N, g/d), urine carbon (U_C, g/d), VS (kg/d) and dVS (kg/d) of lactating cows (n = 1111).

Eq.	Selected model[1]	Model performance[2]			
		RMSPE, %	RSR	MB, %	SB, %
37	$CH_4 = –108.00\ (13.96) + 17.65\ (0.56) \times DMI + 3.04\ (0.40) \times ADF + 25.86\ (1.95) \times mFat – 1.89\ (0.22) \times MY$	16.7	0.54	0.66	4.4
38	$CO_2 = 2.77\ (1.18) + 0.39\ (0.019) \times DMI + 0.077\ (0.033) \times CP$	7.5	0.38	0.58	4.5
39	$Water_{in} = –19.98\ (9.08) + 2.71\ (0.28) \times DMI + 0.35\ (0.11) \times DM + 0.48\ (0.11) \times MY$	42.5	0.91	0.47	1.1
40	$F_{DM} = –0.34\ (1.23) + 0.38\ (0.019) \times DMI – 0.084\ (0.032) \times CP + 0.047\ (0.015) \times ADF$	10.6	0.33	0.13	0.15
41	$F_N = –62.71\ (7.14) + 10.22\ (0.19) \times DMI + 2.00\ (0.33) \times CP + 2.59\ (0.56) \times Lignin$	14.9	0.41	0.14	3.1
42	$F_C = 149.3\ (116.55) + 177.51\ (2.56) \times DMI + 19.93\ (2.29) \times ADF – 42.22\ (4.18) \times CP + 35.27\ (11.36) \times mFat – 111.47\ (19.32) \times mPro$	10.8	0.34	0.18	0.50
43	$F_w = –4.07\ (2.69) + 2.08\ (0.046) \times DMI + 0.42\ (0.036) \times ADF – 0.35\ (0.076) \times CP – 0.068 \times (0.022)\ DM – 0.0076\ (0.0016) \times DIM$	14.7	0.0011	0.23	2.4
44	$U_t = 1.11\ (2.84) + 0.65\ (0.094) \times DMI + 0.71\ (0.14) \times CP – 0.24\ (0.037) \times MY$	47.0	0.92	0.23	3.3
45	$U_N = –242.33\ (11.69) + 9.59\ (0.38) \times DMI +$	20.3	0.47	0.020	7.4

	16.24 (0.49) × CP + 0.053 (0.014) × BW – 2.47 (0.15) × MY				
46	U_C = –215.88 (31.58) + 8.54 (0.84) × DMI + 11.20 (1.35) × CP + 0.14 (0.035) × BW + 10.85 (2.40) × Lignin	35.8	0.83	0.63	0.32
47	VS = –1.56 (1.10) + 0.41 (0.020) × OMI + 0.061 (0.015) × ADF	10.4	0.35	0.84	0.016
48	dVS = –1.25 (1.10) + 0.37 (0.020) × OMI + 0.025 (0.010) × NDF	11.3	0.37	0.73	0.011

[1]Model parameters are reported as posterior means and standard deviation in parenthesis. DMI is in kg/d; CP, NDF, ADF and Lignin are in % of dietary DM; mFat = milk fat, %; mPro = milk protein, %; DM is % of as-fed diet; DIM = day in milk; BW is in kg; OMI = organic matter intake, kg/d.

[2]RMSPE = Root mean square prediction error, expressed as a percentage of observed mean; RSR = Ratio of RMSPE to observed standard deviation; MB = Mean bias, expressed as a percentage of MSPE; SB = Slope bias, expressed as a percentage of MSPE.

Table 9. Selected multivariate model and root mean square prediction error (RMSPE, % of observed mean) for enteric CH_4 (g/d), CO_2 (kg/d), water intake ($Water_{in}$, kg/d), fecal DM (F_{DM}, kg/d), fecal nitrogen (F_N, g/d), fecal carbon (F_C, g/d), fecal water (F_w, kg/d), total urine (U_t, kg/d), urine nitrogen (U_N, g/d), urine carbon (U_C, g/d), VS (kg/d) and dVS (kg/d) of nonlactating cows (n = 591).

Eq.	Selected model[1]	Model performance[2]			
		RMSPE, %	RSR	MB, %	SB, %

49	$CH_4 = 45.43\ (5.99) + 17.84\ (0.48) \times DMI - 2.40\ (1.11) \times EE$	15.9	0.59	1.6	0.58
50	$CO_2 = 2.87\ (1.17) + 0.57\ (0.057) \times OMI$	9.4	0.45	0.21	1.8
51	$Water_{in} = 8.58\ (4.21) + 1.15\ (0.31) \times DMI + 0.91\ (0.35) \times Ash$	60.7	1.0	1.1	0.68
52	$F_{DM} = -1.16\ (1.24) + 0.35\ (0.054) \times DMI + 0.023\ (0.012) \times NDF$	14.9	0.35	0.46	0.37
53	$F_N = -27.14\ (3.35) + 9.11\ (0.18) \times DMI + 1.16\ (0.16) \times CP$	14.7	0.39	1.9	1.6
54	$F_C = -526.36\ (33.35) + 151.36\ (2.56) \times DMI + 19.24\ (0.82) \times ADF$	13.9	0.32	2.5	1.3
55	$F_w = -6.38\ (1.33) + 1.58\ (0.069) \times DMI + 0.20\ (0.021) \times ADF$	21.0	0.42	4.1	0.48
56	$U_t = 8.84\ (2.78) - 0.14\ (0.067) \times ADF + 1.22\ (0.25) \times Ash$	69.8	0.98	1.0	0.0062
57	$U_N = -124.87\ (9.79) + 12.16\ (0.44) \times DMI + 8.15\ (0.44) \times CP + 0.44\ (0.10) \times NDF$	19.1	0.56	8.64	0.36
58	$U_C = 5.68\ (18.13) + 14.54\ (1.54) \times DMI + 3.90\ (1.62) \times Ash$	48.3	0.93	0.53	0.16
59	$VS = -0.84\ (1.24) + 0.36\ (0.058) \times OMI + 0.039\ (0.016) \times ADF$	15.5	0.39	0.97	1.33
60	$dVS = -0.16\ (1.18) + 0.32\ (0.055) \times DMI$	19.2	0.49	3.7	0.077

[1]Model parameters are reported as posterior means and standard deviation in parenthesis. DMI is in kg/d; CP, NDF, ADF, EE and Ash are in % of dietary DM; OMI = organic matter intake, kg/d.

[2]RMSPE = Root mean square prediction error, expressed as a percentage of observed mean; RSR = Ratio of RMSPE to observed standard deviation; MB = Mean bias, expressed as a percentage of MSPE; SB = Slope bias, expressed as a percentage of MSPE.

Table 10. Selected multivariate model and root mean square prediction error (RMSPE, % of observed mean) for enteric CH_4 (g/d), CO_2 (kg/d), water intake ($Water_{in}$, kg/d), fecal DM (F_{DM}, kg/d), fecal nitrogen (F_N, g/d), fecal carbon (F_C, g/d), fecal water (F_w, kg/d), total urine (U_t, kg/d), urine nitrogen (U_N, g/d), urine carbon (U_C, g/d), VS (kg/d) and dVS (kg/d) of heifers (n = 414).

Eq.	Selected model[1]	Model performance[2]			
		RMSPE, %	RSR	MB, %	SB, %
61	$CH_4 = 16.64\ (0.56) \times DMI + 0.86\ (0.12) \times NDF$	19.9	0.63	5.6	0.014
62	$CO_2 = 0.62\ (0.070) \times OMI$	34.1	1.5	94.2	0.12
63	$Water_{in} = 1.69\ (0.23) \times DMI + 0.093\ (0.054) \times DM + 1.18\ (0.27) \times Ash$	82.8	1.1	44.1	2.9
64	$F_{DM} = 0.34\ (0.066) \times DMI$	22.0	0.58	30.2	0.028
65	$F_N = -35.040\ (20.10) + 9.40\ (0.20) \times DMI + 1.17\ (0.17) \times CP + 1.57\ (0.25) \times Lignin + 2.22\ (0.48) \times EE$	16.7	0.43	1.4	1.3
66	$F_C = -369.69\ (42.91) + 160.22\ (2.56) \times DMI + 12.25\ (0.79) \times ADF$	12.7	0.33	0.27	1.5
67	$F_w = -2.75\ (19.80) + 1.38\ (0.075) \times DMI + 0.16\ (0.028) \times ADF - 0.098\ (0.060) \times CP$	26.8	0.60	26.6	0.17

68	U_t = 0.53 (0.11) × DMI + 1.27 (0.13) × Ash	43.9	0.84	10.6	1.5
69	U_N = –71.25 (21.92) + 10.72 (0.43) × DMI + 5.31 (0.35) × CP	23.6	0.49	3.2	6.9
70	U_C = 13.38 (2.12) × DMI	79.8	1.0	12.0	0.21
71	VS = 0.37 (0.066) × DMI	22.7	0.59	4.5	0.0048
72	dVS = 0.36 (0.069) × OMI	23.0	0.60	6.6	0.057

[1]Model parameters are reported as posterior means and standard deviation in parenthesis. DMI is in kg/d; CP, NDF, ADF, EE and Ash are in % of dietary DM; OMI = organic matter intake, kg/d.

[2]RMSPE = Root mean square prediction error, expressed as a percentage of observed mean; RSR = Ratio of RMSPE to observed standard deviation; MB = Mean bias, expressed as a percentage of MSPE; SB = Slope bias, expressed as a percentage of MSPE.

GHG Production

The prediction of enteric CH_4 production (Eqs. 1, 13 and 25) involved DMI for all three animal groups, because DMI provides substrate for microbial fermentation to produce CH_4 (Niu et al., 2018). Dietary structural and non-structural carbohydrate concentrations have an impact on the profile of volatile fatty acids in the rumen (Bannink et al., 2008). Structural carbohydrates are positively correlated with CH_4 production (Moe and Tyrrell, 1979; Bannink et al., 2008), which was represented through the positive coefficients of ADF and NDF in the CH_4 production equations for lactating cows and heifers. However, Eq. 13 did not contain NDF or ADF, indicating other factors might have a more important effect for nonlactating cows. Dietary EE presented in the CH_4 production equation for nonlactating cows had a negative coefficient, which agrees with previous studies showing that inclusion of lipids in the diet has a CH_4 mitigation effect (e.g., Beauchemin et al., 2008; Moate et al., 2011). However, the CH_4 production equation for lactating cows contained MY and mFat instead of EE. The positive coefficient of mFat may be due to the relationship between acetate production and milk fat. Acetate is required for *de novo* milk fat synthesis, and it is also associated with the generation of hydrogen for methanogenesis in the rumen (Moraes et al., 2014). The negative coefficient of MY may be explained by the energy balance between CH_4 emission and milk production, because the carbon in gas energy could be used for milk production if not eructated out as CH_4.

Kirchgessner et al. (1991) reported the estimation of CO_2 production through DMI and BW. However, BW was not present in any CO_2 production equations in this study, probably because the variance of BW was largely captured by DMI. Instead, the CO_2 production equation for lactating cows (Eq. 2) contained CP as a covariate, which contributes to the respiration quotient and consequently affects the CO_2 emission (Pedersen et al., 2008).

Water Intake

Besides DMI, dietary DM and ash were present in the $Water_{in}$ equations (Eqs. 3, 15 and 27), which agrees with the previous study by Appuhamy et al. (2016b). However, the RMSPE of $Water_{in}$ was large, especially for nonlactating cows and heifers (> 60%), indicating a poor model fit. Water consumption of animals is highly dependent on the ambient temperature (Khelil-Arfa et al., 2014), which was not available in our dataset and needs to be considered in future studies.

Manure Excretion

The F_{DM} of lactating cows (Eq. 4) was positively associated with ADF and negatively associated with CP, which suggests that increasing dietary lignocellulose decreases DM digestibility (Van

Soest, 1965) and increases in dietary CP tends to decrease F_{DM} (Broderick, 2003). In the F_{DM} equation for nonlactating cows (Eq. 16), NDF was present instead, probably in a similar role to ADF. However, CP was absent in Eq. 16, which agrees with Wilkerson et al. (1997) that fecal excretion for nonlactating cows is mainly dependent on DMI and dietary NDF level. Nennich et al. (2005) reported an equation to estimate fecal excretion for heifers using DMI and BW, however, we only found a significant effect of DMI on F_{DM} for heifers (Eq. 28).

Increasing dietary CP level can increase nitrogen excretion (Broderick, 2003), which was represented by the positive association of CP with nitrogen excretion (F_N and U_N) for all animal groups. Lignin was positively associated with F_N for lactating cows and heifers (Eqs. 5 and 29), and NDF was positively associated with U_N for nonlactating cows (Eq. 21), which might be due to the inhibition of fiber on digestibility (Lloyd et al., 1961). Previous studies reported a significant effect of BW on nitrogen excretion (Wilkerson et al., 1997; Appuhamy et al., 2014), however, we only found such effect on U_N for lactating cows (Eq. 9). In addition, MY was negatively associated with U_N, suggesting an increase of nitrogen efficiency with increasing MY (Wilkerson et al., 1997). Dietary EE was positively associated with F_N for heifers (Eq. 29), which could be explained by the decrease of CP digestibility due to the increase of EE level (NRC 2001).

Fecal carbon was significantly associated with dietary ADF for all animal groups, and with CP for lactating cows (Eqs. 6, 18 and 30), which agrees with Nousiainen et al. (2009) who reported the positive and negative effects of CP and ADF on feed digestibility. Besides, mFat and mPro were also positively and negatively associated with F_C for lactating cows, respectively, which could be due to the association between indigestible non-fiber carbohydrates and milk compositions (Firkins et al., 2001; Cabrita et al., 2007). Dietary CP and BW were positively associated with U_C for lactating cows (Eq. 10), which agrees with Appuhamy et al. (2014). Increasing CP level is associated with increasing urinary purine, thus increases U_C (Colmenero and Broderick, 2006). The prediction accuracy of U_C was not high for all three animal groups (RMSPE > 35%), especially heifers (RMSPE = 79.8%), probably because there are factors outside the dataset needed to be considered, or a nonlinear model would fit better.

Dietary ADF was positively associated with F_W across all the animal groups (Eqs. 7, 19 and 31). This could be due to the positive association of ADF with saliva input to the rumen, which in turn increases F_W (Appuhamy et al., 2014). Dietary CP content was negatively associated with F_W in the Eqs. 7 and 31, which could be explained by the elevated blood urea concentrations due to increasing CP intake, causing water transfer from gut to blood and ending up with less water in feces (Silanikove and Tadmore, 1989). Dietary DM and DIM were also negatively associated with F_W for lactating cows because less dietary water content tends to decrease F_W, and cows in early lactation excrete less water in feces (Appuhamy et al., 2014).

Dietary CP was positively associated with U_t for lactating cows (Eq. 8), probably due to higher protein level leading to more urine (Gonda and Lindberg, 1994). Dietary sodium and potassium have shown significant effects on the urine output (Bannik et al., 1999; Spek et al., 2012), which could be the reason that dietary ash was present in the U_t equations for nonlactating cows and heifers (Eq. 20 and 32). However, the RMSPE of U_t for all animal groups was quite high (> 40%). Given U_t is directly affected by $Water_{in}$, the absence of air temperature could lower the prediction accuracy for both variables.

Manure VS and dVS were predicted through feed intake (DMI or OMI) and structural carbohydrates (NDF or ADF), which is consistent with the negative relationship of dietary structural carbohydrates with feed digestibility (Lloyd et al., 1961). However, Eqs. 24, 35 and 36 included feed intake as the only covariate, which might be due to the higher NDF level in the diet and smaller DMI of nonlactating cows and heifers so that two covariates confounded with each other.

Multivariate vs. univariate models

The results of both the coefficient estimation and cross validation were very close between multivariate and univariate models for all the animal groups. The difference between multivariate and univariate models is that multivariate models included the variance covariance between traits of study and animal random effects, while univariate models only considered the variance. For the ease of visualization, covariances were converted to correlations and are shown in Figures 4 and 5 for animal and study random effects, respectively. The average magnitude (i.e., the absolute value) of pairwise study effect correlations was 0.13 for lactating cows, 0.11 for nonlactating cows and 0.040 for heifers, and the average magnitude of pairwise animal effect correlations was 0.10 for lactating cows, 0.066 for nonlactating cows and 0.076 for heifers. The results indicate that covariances were relatively small compared to variance in this study, therefore the benefits of multivariate modeling were not obvious. Multivariate models have shown a superiority in some genetic studies (Calus and Veerkamp, 2011; Jia and Jannink, 2012), but only when the genetic correlation between traits is high (> 0.5).

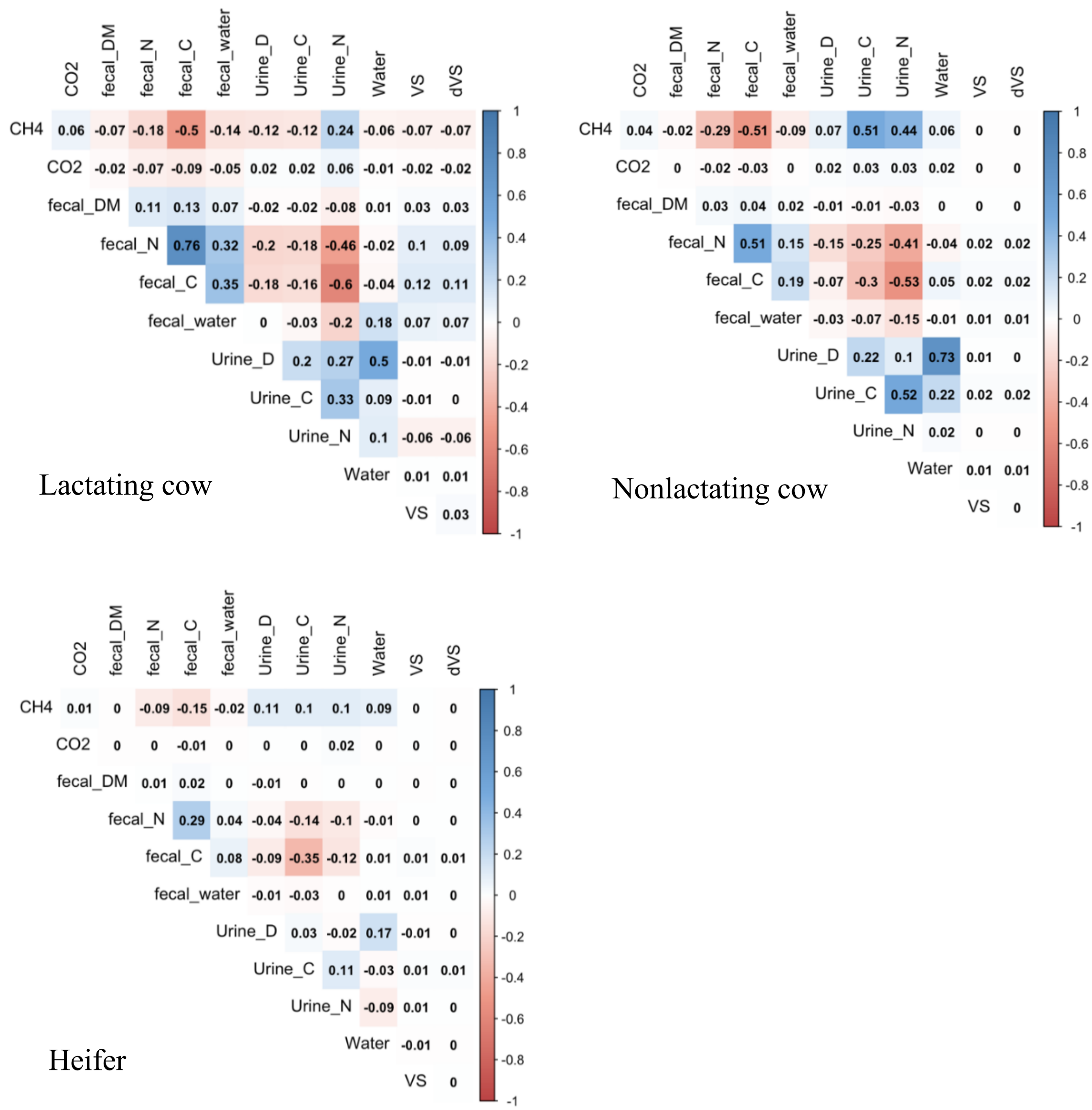

Figure 4. Heatmaps of pairwise correlations of animal random effects among CH4 (g/d), CO2 (kg/d), milk yield (MY, kg/d), water intake (Waterin, kg/d), fecal DM (FDM, kg/d), fecal nitrogen (FN, g/d), fecal carbon (FC, g/d), fecal water (FW, kg/d), total urine (Ut,

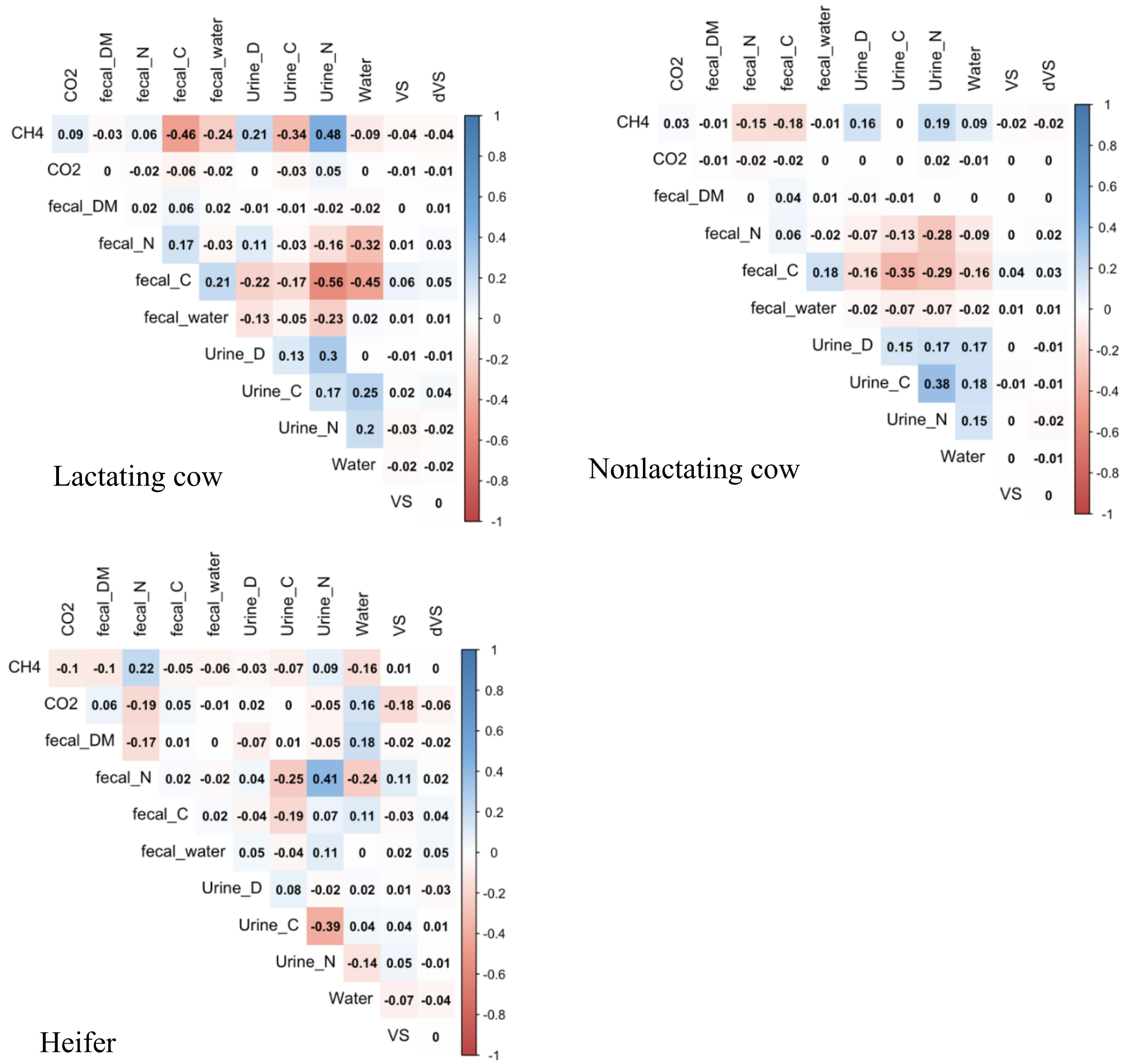

Figure 5. Heatmaps of pairwise correlations of study random effects among CH_4 (g/d), CO_2 (kg/d), milk yield (MY, kg/d), water intake ($Water_{in}$, kg/d), fecal DM (F_{DM}, kg/d), fecal nitrogen (F_N, g/d), fecal carbon (F_C, g/d), fecal water (F_W, kg/d), total urine (U_t, kg/d), urine nitrogen (U_N, g/d), urine carbon (U_C, g/d), VS (kg/d) and dVS (kg/d) for lactating cows, nonlactating cows and heifers.

Comparison of the CH_4 emission model with existing models

Three existing prediction equations of CH_4 emission for lactating cows were compared with the one developed in this study (Eq. 1). The univariate and multivariate models were similar, so only multivariate models were included in the comparison. The equation from Moraes et al. (2014) was selected because it was also developed using the data from US. Appuhamy et al. (2016a) evaluated 40 CH_4 equations for different regions, from which we selected the one (Moate et al., 2011) ranking third in North America. Performance of the top three equations was close. The top two equations were not included because they require fatty acid as a model input, which was not available in our dataset. Niu et al. (2018) developed CH_4 emission equations for different regions using an intercontinental dataset, and we selected the one performing the best in the US.

The prediction accuracy of the three existing equations and the one developed in the current study is shown in Table 11. Our equation performed similarly to the one from Niu et al. (2018), but better than the one from Moate et al. (2011). Although the RMSPE of the equation from Moraes et al. (2014) was the smallest, MB and SB were much larger, especially MB, which indicates that the intercept did not fit well with the dataset. Overall, the CH_4 emission equation for lactating cows developed in this study showed a decent prediction accuracy compared to three existing equations given the independent test dataset. We were only able to examine CH_4 emission for lactating cows due to the lack of other data. The prediction accuracy of other equations should be examined using a comprehensive dataset in future studies. The accuracy of prediction for dry cows by CADEM needs to improve with more data.

Table 11. Prediction accuracy of CH_4 emission for lactating cows using the equation developed in this study and three existing equations.

Eq.	Model performance[1]			
	RMSPE, %	RSR	MB, %	SB, %
(1) This study	36.5	1.1	0.71	16.4
(a) Niu et al. (2018)	36.6	1.1	6.8	8.9
(b) Moate et al. (2011)	43.4	1.3	24.3	16.9
(c) Moraes et al. (2014)	22.9	2.0	60.1	19.9

[1]RMSPE = Root mean square prediction error, expressed as a percentage of observed mean; RSR = Ratio of RMSPE to observed standard deviation; MB = Mean bias, expressed as a percentage of MSPE; SB = Slope bias, expressed as a percentage of MSPE.

Simulation of the Effects of Feed Additives on Mitigating CH_4 Flux from Cattle

In addition to developing CADEM to predict GHG emissions and manure excretion from dairy cattle more accurately, the project team has discussed developing CADEM to simulate mitigation of feed additives on enteric CH_4 flux. A series of equations developed by UCD (Dijkstra et al. 2018; Feng and Kebreab, 2020; Feng et al., 2020) have been incorporated into CADEM to calculate effects of two type feed additives (3-nitrooxypropanol (3NOP) and nitrate) on enteric CH_4 flux mitigation for both dairy and beef cattle.

3-nitrooxypropanol

Following from the previous CARB project (Contract # 17RD018), we started working on 3NOP as the feed additive with the most potential application. Dijkstra et al. (2018) conducted a meta-analysis on CH_4 mitigating effects of 3NOP. The meta-analysis was updated in this project by adding data from Martinez-Fernandez et al. (2018) (beef; 1 study), Vyas et al. (2018) (beef; 2 studies), Kim et al. (2019) (beef; 2 studies), Van Wesemael et al. (2019) (dairy; 2 studies), Melgar et al. (2020a) (dairy; 1 study), Melgar et al. (2020b) (dairy; 6 studies), Melgar et al. (2021) (dairy; 1 study), Aleum et al. (2021) (beef, 3 studies), Schilde et al. (2021) (dairy; 2 studies) and Zhang et al. (2021) (beef; 2 studies). The updated forest plots for Standardized Mean Difference of CH_4 production and yield are shown in Figure 6 and Figure 7.

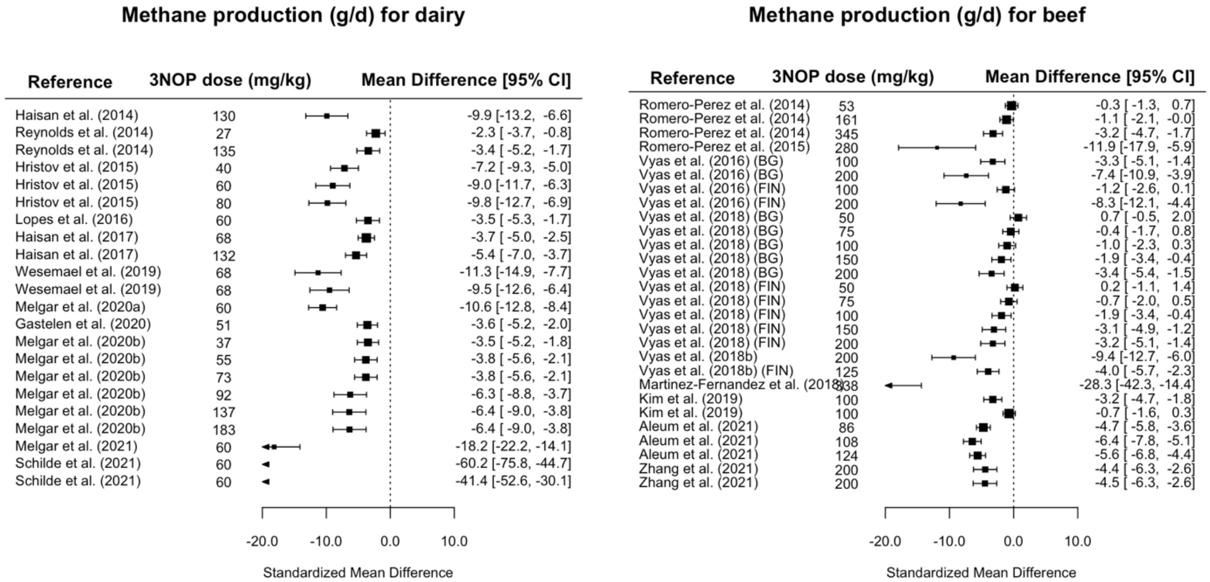

Figure 6. Forest plot showing 3NOP dose (mg/kg of DM) and standardized mean difference (mean difference = 3NOP treatment mean − control treatment mean) in CH4 production (g/d) for beef and dairy cattle studies.

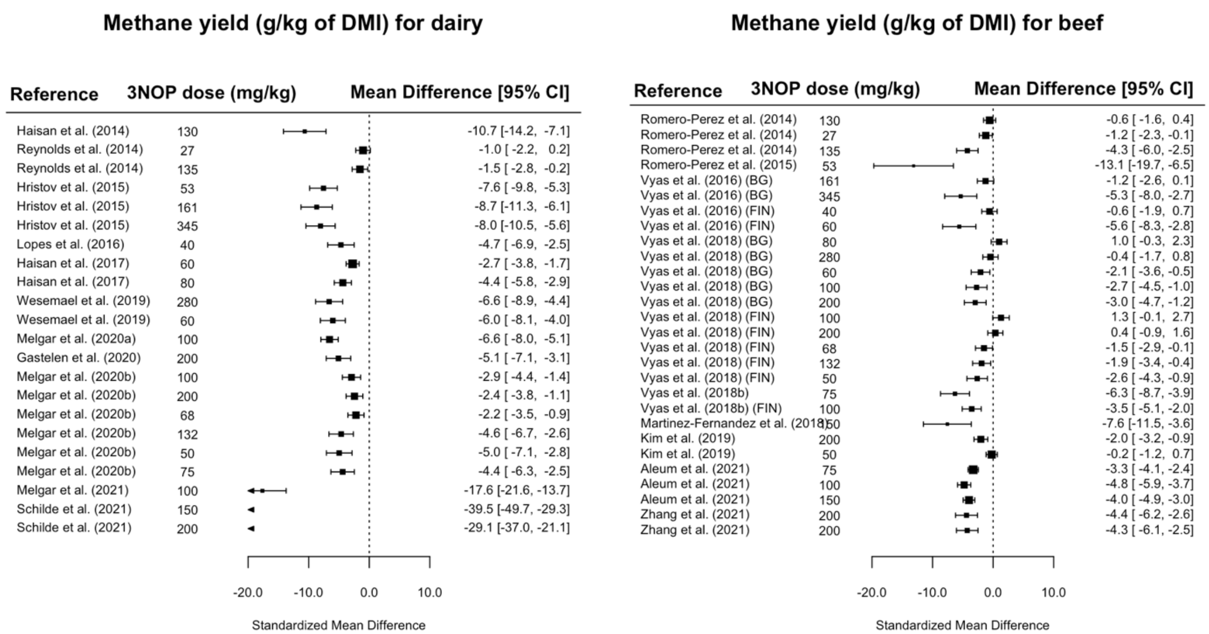

Figure 7. Forest plot showing 3-nitrooxypropanol (3NOP) dose (mg/kg of DM) and standardized mean difference (mean difference = 3NOP treatment mean − control treatment mean) in CH4 yield (g/kg of DMI) for dairy and beef cattle studies.

The results of the mixed-effect models for CH_4 production and yield were similar to the previous study, which indicated effectiveness of 3NOP at mitigating CH_4 emissions (Table 12). As expected, the effect was positively associated with dose, and negatively associated with NDF. Moreover, 3NOP had stronger anti-methanogenic effects in dairy cattle than in beef cattle. The mean value of 3NOP dose was 118 mg/kg of DM, which was slightly lower compared to the 123 mg/kg of DM in previous analysis. The overall mitigating effect of 3NOP was 30.6% at 118 mg/kg inclusion level. In dairy cattle, the impact was 37.7% reduction while in beef cattle it was 26.3% (Table 12).

Table 12. Estimates of overall 3-nitrooxypropanol (3NOP) effect size and of explanatory variables from random- and mixed-effect models for relative mean difference (MD, %) in CH_4 production (g/d) and yield (g/kg of DMI)

Variable and model	CH_4 production			CH_4 yield		
	Mean	SE	*P*-value	Mean	SE	*P*-value
Random-effect model						
Overall 3NOP effect size	-30.57	2.91	< 0.0001	-27.13	2.89	< 0.0001
Mixed-effect model with 3NOP dose as the only covariate						
Overall NOP effect size	-30.47	2.69	< 0.0001	-27.13	2.64	< 0.0001
NOP dose (mg/kg of DM)	-0.11	0.036	0.0017	-0.12	0.036	0.0010
Final mixed-effect model						
Dairy cattle overall NOP effect size	-38.18	3.33	< 0.0001	-34.86	3.43	< 0.0001
Beef cattle overall NOP effect	-26.05	2.76	< 0.0001	-21.07	2.99	< 0.0001

size						
NOP dose (mg/kg of DM)	-0.23	0.034	< 0.0001	-0.22	0.036	< 0.0001
NDF content (g/kg of DM)	0.15	0.022	< 0.0001	0.12	0.025	< 0.0001

The following formula was developed in order to integrate the effect of 3NOP on enteric CH_4 mitigation of dairy cattle in CADEM:

$$CH_4\ reduction = max((-38-0.23\times(3NOP-118)+0.15\times(NDF-333)), -60\%) \quad (73)$$

For beef cattle, the following equation was used in CADEM:

$$CH_4\ reduction = max((-26.1-0.23\times(3NOP-118)+0.15\times(NDF-333)), -81.0\%) \quad (74)$$

where: *CH_4 reduction* = enteric CH_4 reduction per day (%), *3NOP* = 3-nitroxypropanol dose (mg/kg of DM) and *NDF* = dietary neutral detergent fiber concentration (g/kg of DM).

Nitrate

Effect of nitrate on enteric CH_4 mitigation of dairy cattle was incorporated into CADEM using the equation developed by Feng and Kebreab (2020) from previous CARB project (Contract # 17RD018):

$$CH_4\ reduction = max((-20.4-0.911\times(Nitrate-16.7)+0.691\times(DMI-11.1)), -27.6) \quad (75)$$

The effect of nitrate on enteric CH_4 mitigation of beef cattle was integrated as follows:

$$CH_4\ reduction = max((-10.1-0.911\times(Nitrate-16.7)+0.691\times(DMI-11.1)), -29.4) \quad (76)$$

where: *CH_4 reduction* = enteric methane reduction per day (%), Nitrate = nitrate dose (g/kg of DM) and DMI = dry matter intake (kg/day).

Integration of UCD Model with Manure-DNDC in CADEM

We have integrated the UCD enteric model into CADEM to predict GHG emissions and manure excretion from dairy cattle. The model integration processes included coding the empirical equations (Table 2), developing new GUI to read input parameters, converting the input parameters to the parameters in the equations, reporting enteric GHG emissions, and linking manure excretion with processes of simulating manure transfers and transformation. In order to check if the UCD fermentation model has been error-freely incorporated into CADEM, we compared simulations from CADEM and outputs from the UCD fermentation model. The compared variables included CO_2 flux, CH_4 flux, urine C and N productions, fecal C and N productions, total urine production, and fecal water production. We collected relevant animal and feed information, and estimated CADEM input parameters based on this information. In total, 65 cases were evaluated for each variable. The simulations of these variables between CADEM and the UCD fermentation model were very close (Figure 8 and Figure 9). These results indicate that the UCD fermentation model for calculating GHG emissions from dairy cattle and manure excretion were correctly incorporated into CADEM.

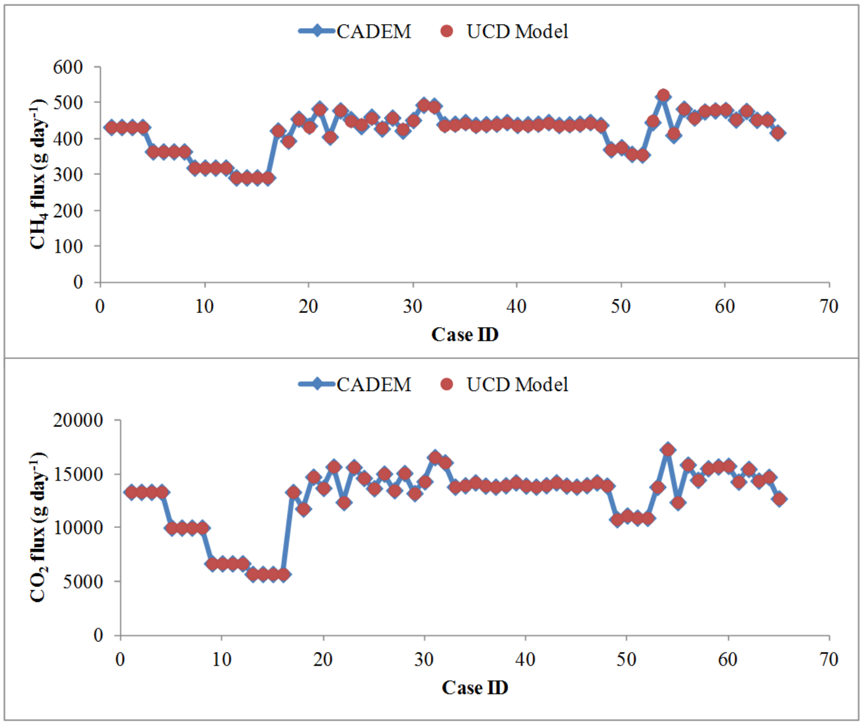

Figure 8. Comparisons in CH_4 and CO_2 fluxes between CADEM simulations and outputs from the UCD model.

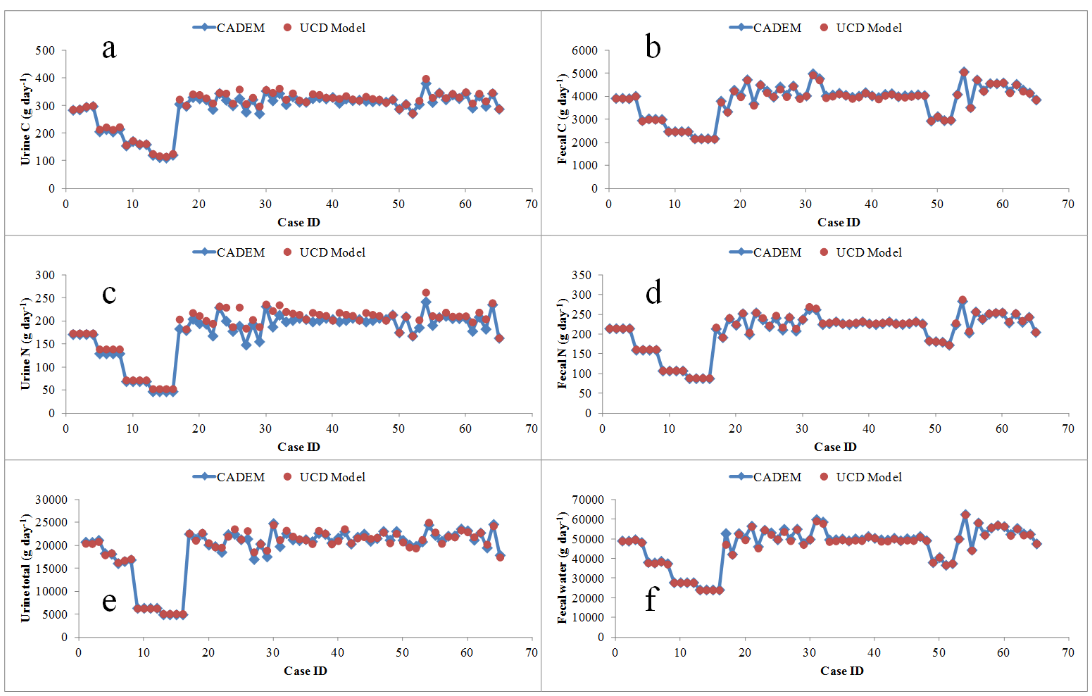

Figure 9. Comparisons in productions of (a) urine C, (b) fecal C, (c) urine N, (d) fecal N, (e) total urine, and (f) fecal water between CADEM simulations and outputs from the UCD model.

Expand CADEM to Simulate C, N, and P Dynamics of Multiple Slurry Manure Storage Areas

In order for CADEM to simulate GHG and N gas fluxes from major components within California dairy farms and to better represent conditions of California dairies, we have also improved CADEM's processes of simulating water, C, N, and P dynamics in slurry manure storage areas. The original version of Manure-DNDC can simulate only one slurry storage area (e.g., single lagoon), although there are often multiple slurry storage areas in real dairy farms in California. Furthermore, the Manure-DNDC model cannot simulate slurry storage areas that are operated in series (i.e., a downstream slurry storage area receives water, C, N, and P outputs from an upstream slurry storage area), although this management practice is common in California dairies. In order to improve the model's flexibility and applicability in simulating California dairy farms, we have incorporated new processes to simulate transfers and interactions of water, C, N, and P between two slurry storage areas on a daily basis. The water, C, N, and P of an upstream slurry storage area can be loaded into a downstream slurry storage area and can influence manure transformation, GHG and N gas productions, and other biogeochemical processes of the downstream slurry storage areas. This new function would enable CADEM to simulate two slurry storage areas that are operated in series, such as the structure with a setting basin followed by manure storage lagoon. The old interface (Figure A3a) has also been updated to allow users to set input parameters (e.g., climate, properties, and manure management practices) of different slurry storage areas (Figure A3b).

In addition to simulating transfers and interactions of water, C, N, and P between two slurry storage areas, the CADEM has been expanded to comprehensively simulate transfers and interactions of water, C, N, and P among major components in a dairy farm, including housing, slurry manure storage areas, compost, digesters, and crop fields with manure amendments. Specifically, new processes to simulate transfers and interactions of water, C, N, and P between slurry storage areas and other components (i.e., housing, digester, crop fields) within a dairy farm have been incorporated (Figure 10). With these new processes, the model can simulate manure transfers among these components (e.g., removal of manure from housing to multiply slurry storage areas, manure transfers from slurry storage areas to digester, compost, and/or crop field) and impacts of manure transfers on water, C, N, and P dynamics in each component.

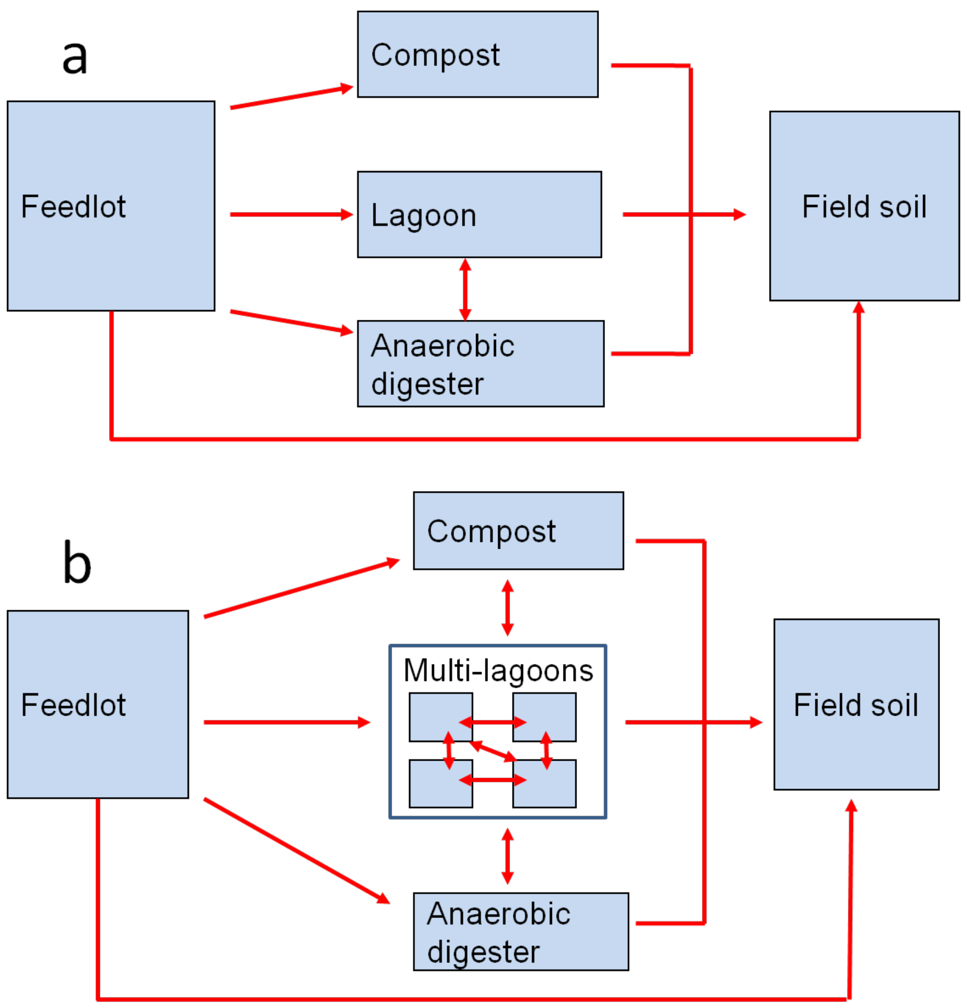

Figure 10. Old (a) and new (b) framework of simulating manure transfers among different components in a dairy farm.

Processes to distinguish liquid and solid fractions of manure during manure transfers were also added in CADEM, so that liquid and solid manure could be transferred among farm components in different amounts. The liquid fraction of manure contains free water and dissolved organic C and nutrients, including urea, ammonium, and nitrate. The solid fraction of manure contains non-dissolved organic C and P. For example, model users can set more liquid fraction than solid fraction when transferring manure from digester to slurry storage areas. The CADEM can also distinguish solid and liquid fractions of manure that transfers from housing and/or manure storage areas to fields. For example, the CADEM can simulate the scenario that one field receives all liquid manure while another field receives all solid manure from manure storage areas. The original Manure-DNDC can only simulate the scenario of receiving bulk manure including both solid and liquid fractions. These new functions provide more flexibility in tracking changes of manure characteristics during manure transfers and improve simulations of water, C, N, and P dynamics in farm components.

Several old interfaces have also been updated. The new developed interfaces allow model users to set input parameters (e.g., lagoon properties and manure management practices) of different slurry storage areas (Figure A4), removal of manure from housing to multiple slurry storage areas (Figure A5), manure transfers between digester and slurry storage areas (Figure A6), and remove liquid and solid fractions of manure applied into crop fields (Figure A7).

Model Validation

We have reviewed reports and papers from relevant studies to identify field data that can be used to improve, calibrate, and validate CADEM. We have focused on field data of emissions of GHG and N gas from dairy cattle and farm components or manure properties. Through this project, we have compiled comprehensive observations of CO_2 and CH_4 emissions and manure excretion (including total manure as well as C and N amounts in manure) from dairy cattle (Liu et al., 2016; Moraes et al., 2014; Roque et al., 2019; Tewoldebrhan et al., 2017). The dataset includes over 1100 (1121 to 1436) data points for each variable and represents different animal and feeding conditions and does not include data used to develop enteric methane equations. The dataset also includes relevant model input information of dairy cattle and feeding properties.

We have tested CADEM simulations of CO_2 and CH_4 emissions, productions of total urine and urine C and N, and productions of total fecal and fecal C and N from dairy cattle against these field observations. The simulations of GHG emissions from manure have not been evaluated because field observations with adequate frequency and some relevant model input parameters were not available. The CADEM was driven by animal and feeding input parameters, including DMI, DM, MPR, BW, DIM, CP, ADF, and NDF. The simulations of CO_2 flux, CH_4 flux, productions of total urine and urine C and N, and productions of total fecal and fecal C and N were compared against corresponding field observations (Figure 11 to Figure 14). We used zero-intercept linear regression between simulations and observations to evaluate CADEM performance. The slope of the regression indicates the consistency between simulations and observations (Moriasi et al., 2007). In addition, two statistical indices, the relative root mean squared error (RRMSE) and the coefficient of correlation (R), were used to quantity the accordance and correlation between model predictions and field observations (Moriasi et al., 2007).

$$RRMSE = \frac{100}{|\overline{o}|}\sqrt{\frac{\sum_{i=1}^{n}(p_i\text{-}o_i)^2}{n}} \qquad (77)$$

$$R = \frac{\sum_{i=1}^{n}(o_i - \overline{o})(p_i - \overline{p})}{\sqrt{\sum_{i=1}^{n}(o_i - \overline{o})^2 \sum_{i=1}^{n}(p_i - \overline{p})^2}} \qquad (78)$$

where, o_i and p_i are the observed and simulated values, respectively; and are their averages; and n is the number of values.

The means and ranges of CADEM simulations were 348 (160 to 628) g head^{-1} day^{-1} for CH_4 flux, 9659 (1310 to 22770) g head^{-1} day^{-1} for CO_2 flux, 231 (40 to 370) g head^{-1} day^{-1} for urine C, 149 (30 to 280) g head^{-1} day^{-1} for urine N, 17526 (9431 to 25844) g head^{-1} day^{-1} for total urine, 2498 (250 to 4680) g head^{-1} day^{-1} for fecal C, 147 (20 to 270) g head^{-1} day^{-1} for fecal N, and 29293 (534 to 58376) g head^{-1} day^{-1} for total fecal. The means and ranges of field observations were 315 (30 to 688) g head^{-1} day^{-1} for CH_4 flux, 10853 (3532 to 18946) g head^{-1} day^{-1} for CO_2 flux, 241 (12 to 707) g head^{-1} day^{-1} for urine C, 165 (28 to 397) g head^{-1} day^{-1} for urine N, 18550 (4382 to 58895) g head^{-1} day^{-1} for total urine, 2485 (238 to 5208) g head^{-1} day^{-1} for fecal C, 151 (17 to 441) g head^{-1} day^{-1} for fecal N, and 31814 (2054 to 74832) g head^{-1} day^{-1} for total fecal. The means and ranges of the simulations were comparable with the corresponding observations for each evaluated variable.

Table 13. The model performance in simulating CO_2 and CH_4 emissions, productions of total urine and urine C and N, and productions of total fecal and fecal C and N from dairy cattle

Variables	Slope	RRMSE, %	R
CH_4	1.04	20%	0.79

CO_2	0.90	13%	0.87
Urine C	0.92	19%	0.80
Urine N	0.85	21%	0.89
Total Urine	0.87	36%	0.59
Fecal C	0.98	9%	0.94
Fecal N	0.93	16%	0.90
Total Fecal	0.91	16%	0.94

The slopes of the zero-intercept linear regression lines and the RRMSE values between the simulations and observations were 1.04 and 20% for CH_4 emission, 0.90 and 13% for CO_2 emission, 0.92 and 19% for urine C, 0.85 and 21% for urine N, 0.87 and 36% for total urine, 0.98 and 9% for fecal C, 0.93 and 16% for fecal N, and 0.91 and 16% for total fecal, respectively (Table 13, Figures 11 to 14). The R values between the simulations and observations ranged from 0.59 to 0.94 among these variables, and the simulations were significantly correlated with the corresponding observations for all the evaluated variables (Table 13, Figures 11 to 14). These results indicate a general agreement between the simulated and observed CO_2 flux, CH_4 flux, productions of total urine and urine C and N, and productions of total fecal and fecal C and N, although the goodness of fit varied across the variables.

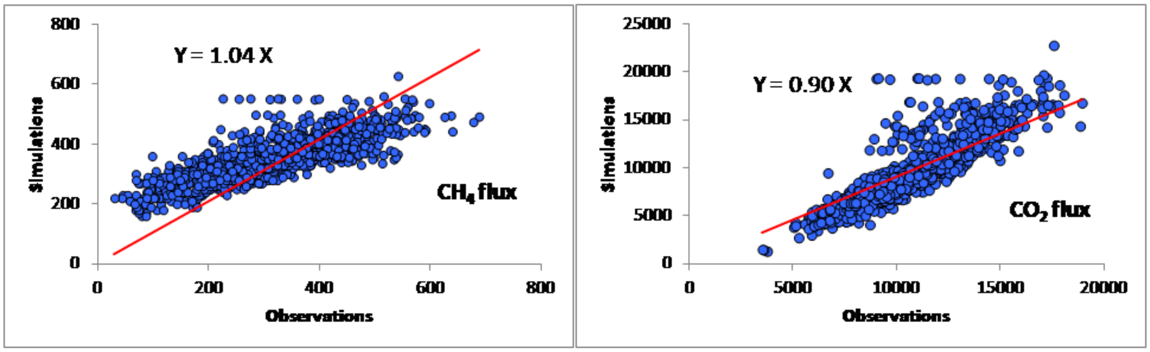

Figure 11. Comparison of simulated and observed (a) CH_4 flux (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.79, *P* < 0.01, *n* = 1436). (b) CO_2 flux (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.87, *P* < 0.01, *n* = 1310).

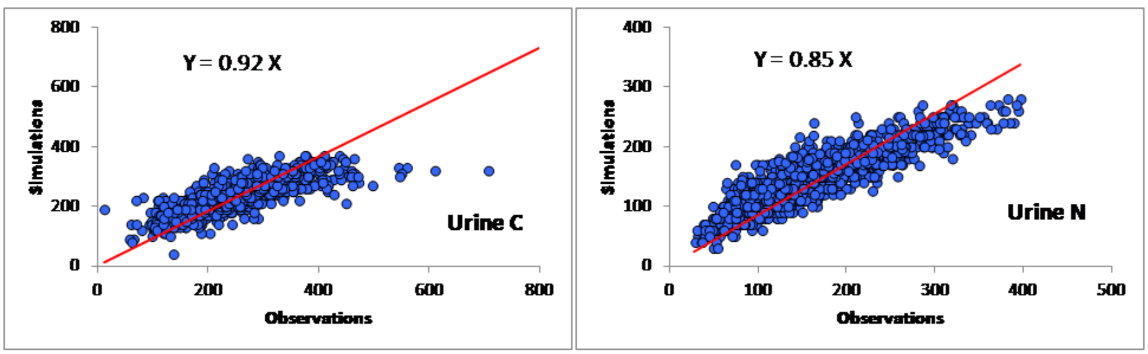

Figure 12. Comparison of simulated and observed (a) urine C (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.80, *P* < 0.01, *n* = 1204). (b) urine N (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.89, P < 0.01, n = 1289).

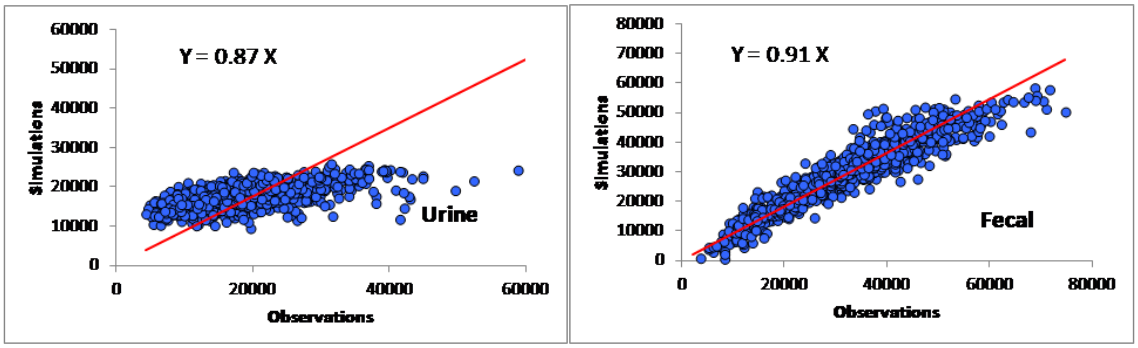

Figure 13. Comparison of simulated and observed (a) total urine (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.59, $P < 0.01$, $n = 1138$). (b) total fecal (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.94, $P < 0.01$, $n = 1121$).

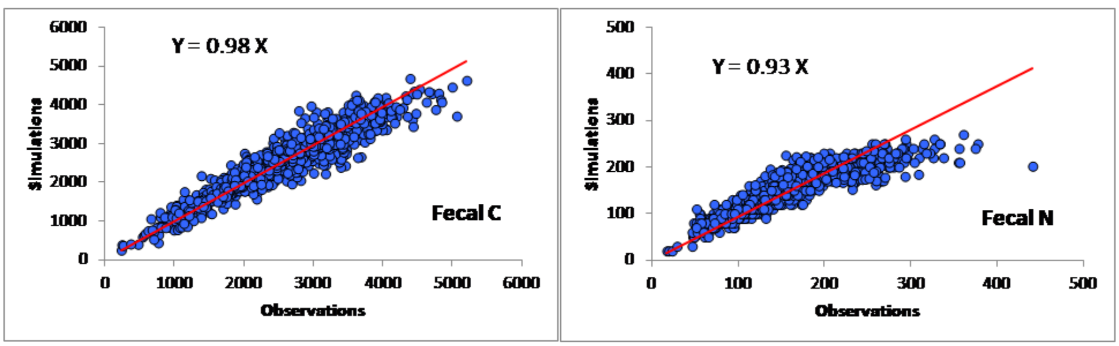

Figure 14. Comparison of simulated and observed (a) fecal C (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.94, $P < 0.01$, $n = 1143$). (b) fecal N (unit: g head^{-1} day^{-1}) from dairy cattle. The function shown describes the zero-intercept fitted regression line. The correlation between simulations and observations is significant (R = 0.90, $P < 0.01$, $n = 1289$).

Overall, these model evaluations confirmed that the new equations from the UCD fermentation model have been successfully incorporated. By including these new equations, the CADEM can reliably predict CO_2 and CH_4 emissions from enteric fermentation, productions of total urine and urine C and N, and productions of total fecal and fecal C and N from dairy cattle.

Farm-Scale Simulations

Using the new developed CADEM, farm-scale simulations were performed to demonstrate the capability of CADEM to simulate C and N dynamics as well as GHG and NH_3 emissions from major components of a real dairy farm in Kern County. The target farm consisted of animal housings, solid manure piles, two lagoons used for manure storage, and crop fields where manure was applied. The animal housings totally held 6076 dairy cows on average, including 2959 milk cows (average weight: 1400 lb), 636 dry cows (average weight: 1450 lb), 932 bred heifers (15 to 24 month) (average weight: 1000 lb), 1191 heifers (7 to 14 month to breeding) (average weight: 300 lb), and 358 calves. The feeding information was not available. We therefore set the feeding input parameters by referring to the studies used for model tests. Specifically, average feeding rate was set as 24.0 kg DM head^{-1} day^{-1} for milk cows, 24.0 kg DM head^{-1} day^{-1} for dry cows, 17.0 kg DM head^{-1} day^{-1} for bred heifers (15 to 24 month), 5.0 kg DM head^{-1} day^{-1} for heifers (7 to 14 month to breeding), and 5.0 kg DM head^{-1} day^{-1} for calves. The CP content was set as 14% for all types of cows.

All model input parameters, including climate, dairy cattle, housing, manure storage areas, crop fields, soil, cropping system, and management practices, were set to represent the environmental conditions, farm components, and management practices in this farm. Most of these input parameters were estimated by referring to dairy annual report in 2018 and dairy waste management plan in California (personal communication with CARB staff). The lagoons were uncovered, and had a surface area of around 10000 m^2 and a maximum storage capacity of around 52000 m^3. Because there is no information about the manure amount transferred from housing to each lagoon (i.e., partitions of the manure between two lagoons) and the surface area and maximum storage capacity of the two lagoons are similar, we assumed that these lagoons received identical manure from the animal housings each day. Based on the dairy annual report, the slurry manure stored in the lagoon was removed ten times annually and applied to the surface of the crop fields (around 246 ha) as wastewater before planting or during crop growing seasons. The crop fields were planted with triticale during winter and with corn silage during summer. The crop fields received manure application eleven times annually (dry manure: one time; wastewater: ten times). The local soil properties were determined based on the SSURGO database from the Natural Resources Conservation Service, U. S. Department of Agriculture (NRCS, 2022). We used the soil properties of the soil with the largest coverage in the target farm. The soil was a sandy loamy with clay content 0.13, pH (H_2O) 8.2, bulk density 1.55 g cm^{-3}, and content of soil organic carbon 0.004 kg C kg^{-1} soil dry weight based on the SSURGO database. In addition to manure management, input parameters of other farming management practices are required to run CADEM at a farm scale. These input parameters included planting and harvest dates, tillage, fertilization, and irrigation, and were primarily estimated from field records in dairy annual report in 2018.

Five scenarios with different manure management practice assumptions were simulated to investigate the impacts of each management practice on GHG and NH_3 emissions. In the baseline scenario (SB), it was assumed that the manure on the housing floors was removed by a scraper on a daily basis. It was also assumed that 25% of solid manure and 80% of liquid manure was transferred into the lagoons and the rest of the solid and liquid manure was transferred into the solid manure piles. The manure stored in the solid piles was removed four times annually, with most (around 95%) of the removed manure sold to market and therefore removed out of the target farm, and a small fraction (around 5%) of the removed manure applied to the crop fields. In the first scenario (S1), the manure was assumed to be flushed with water (10 gallons hd^{-1} day^{-}

^{1}), while other input parameters were identical to SB. In the second and third scenarios (S2 and S3), the fraction of housing manure transferred to the lagoons was different from SB. Specifically, the solid manure transferred to the lagoons increased from 25% to 50% for the S2, and all the housing manure was transferred to the lagoons and there was no solid manure pile for the S3. The forth scenario (S4) was similar to SB except that the manure stored in the solid piles were removed two times annually with 50% of the manure applied into fields and 50% of the manure remained in the piles each time (S4).

CADEM was run for 2017 and 2018 under the four scenarios, with the simulations in 2017 used for model initialization. Daily meteorological data (i.e., maximum and minimum air temperatures, precipitation) in 2017 and 2018 were derived from weather data produced by the DAYMET model (Thornton et al., 2022) to support the simulations. The modeled NH_3 and GHG emissions from each farm component and the whole farm in 2018 were used for analysis.

Results of the baseline scenario

Table 14 lists the simulated GHG and NH_3 emissions from the housings (including both animal and housing floor), solid manure piles, lagoons, and crop fields under different scenarios. The rates of annual total C and N excretions were 6443.6 metric ton (MT) C yr^{-1} and 592.9 MT N yr^{-1}, respectively, under SB.

The rates of annual total CO_2 emissions from the housings, solid manure piles, lagoons, and crop soils were 6073.7, 336.9, 186.6, and 589.0 MT C yr^{-1}, respectively. At the farm scale, the rate of CO_2 emissions from animals, manure, and soils (i.e., soil heterotrophic respiration) was 7186.1 MT C yr^{-1} in 2018 (Table 14). The housings, including dairy cattle and manure in housings, were simulated as the largest source of CO_2 emissions, contributing to about 85% of the annual total CO_2 emissions under SB. However, we note that the simulated total CO_2 emissions were not net

CO_2 exchanges between the atmosphere and the simulated farm because not all CO_2 exchanges (e.g., crop photosynthesis and respiration, SOC sequestration due to external manure or residue inputs) were included into these results.

The rates of annual total CH_4 emissions from the housings, solid manure piles, lagoons, and crop soils were 657.7, 0, 177.1, and 0 MT C yr^{-1}, respectively, under SB. At the farm scale, the rate of CH_4 emissions was 834.9 MT C yr^{-1} in 2018 (Table 14). The housings, including cattle enteric emissions and manure in housings, were simulated as the largest source of CH_4 emissions, contributing to about 79% of the annual total CH_4 emissions. The simulated CH_4 emission was zero for the solid manure pile and crop fields because of their aerobic conditions that is assumed not suitable for CH_4 production in the DNDC model (Deng et al., 2017).

The rates of annual total N_2O emissions from the housings, solid manure piles, lagoons, and crop soils were 8.6, 1.4, 0.7, and 3.3 MT N yr^{-1}, respectively, under SB. At the farm scale, the rate of N_2O emissions was 14.0 MT N yr^{-1} in 2018 (Table 14), an amount that comprises 2.4% of the excreted N. The housings were simulated as the largest source of N_2O emissions, contributing to about 61% of the annual total N_2O emissions of the simulated dairy farm. The housings were simulated as the largest source of N_2O because we assumed that the manure in the housings was removed by scraper and there was manure accumulation on the housing floors. In addition, the area of the fields receiving manure was not large and most of solid manure was removed out of the simulated system, which contributed to the relatively low N_2O emissions from the fields.

The rates of annual total NH_3 emissions from the housings, solid manure piles, lagoons, and crop fields were 50.3, 53.6, 62.6, and 38.4 MT N yr^{-1}, respectively. At the farm scale, the rate of NH_3 loss was 204.9 MT N yr^{-1} in 2018, an amount that comprises 35% of the excreted N.

Comparison of the emissions under different scenarios

Compared to SB, removing the manure by flushing the housings with water (S1, Table 14) decreased the N_2O emissions from the housings and solid manure piles by 51% (4.2 vs. 8.6 kg N head^{-1} yr^{-1}) and 41% (0.8 vs. 1.4 kg N head^{-1} yr^{-1}), respectively, primarily because of the wetter conditions under the water flushing. The wetter conditions restricted nitrification and thereby N_2O productions from nitrification in the housings and solid manure piles. This scenario increased the CO_2 and NH_3 emissions from the solid manure piles (Table 14) primarily because the wetter conditions were favorable for decomposition and productions of CO_2 and NH_4^+ that is a substrate for NH_3 production.

In comparisons with the baseline scenario, transferring more housing solid manure (50% vs. 25%) into the lagoons (S2) increased the CO_2, CH_4, and NH_3 emissions from the lagoons by 57%, 59%, and 14%, respectively, because of the more organic manure transferred into the lagoons, which provided more substrates for CO_2 and CH_4 productions (Table 14). Increasing the fraction of manure transferred to the lagoons to 100% (S3) further increased the CO_2, CH_4, and NH_3 emissions from the lagoons by 183%, 187%, and 64%, respectively, in comparison with the baseline scenario. Lagoons contributions to total CH_4 emissions increased from 21% under SB to 30% under S2 and to 44% under S3. These practices did not substantially increase the N_2O emissions from the lagoons because the anaerobic conditions, instead of the substrates, were the limiting factor for N_2O production in the lagoons.

Applying more manure stored in the solid piles into the fields (S4, Table 14) substantially increased the CO_2, N_2O, and NH_3 emissions from the fields by 2.6 folds, 2.1 folds, and 47%, respectively, because of the more organic manure transferred into the fields. Again, we note that the simulated total CO_2 emissions were not net CO_2 exchanges between the atmosphere and the simulated farm.

The simulated CH_4 emissions (around 144 kg CH_4 hd^{-1} yr^{-1}) from housings (including both animal and housing floor) were comparable with the CH_4 emissions (enteric CH_4 emission: around 120 kg CH_4 hd^{-1} $year^{-1}$, barn CH_4 emission: 33±19 kg CH_4 hd^{-1} $year^{-1}$) estimated based on reviewing field studies (Owen and Silver, 2014). The simulated CH_4 emissions from the lagoons ranged between 11.6 and 33.9 kg CH_4 m^{-2} yr^{-1} under the different scenarios, which were comparable with the reported CH_4 emissions (20±5 kg CH_4 m^{-2} yr^{-1}) per lagoon area (Owen and Silver, 2014). However, the simulated lagoon CH_4 emissions per head animal (38.3 to 111.7 kg CH_4 hd^{-1} yr^{-1}) were lower than the corresponding field data (368±193 kg CH_4 hd^{-1} yr^{-1}) (Owen and Silver, 2014). The different lagoon CH_4 emissions between per lagoon area and per head animal and under different scenarios suggested that both lagoon characteristics (such as lagoon area) and manure management practices may affect lagoon CH_4 emissions. The housings were simulated as the largest source of N_2O emissions all scenarios excepting S4. This result is different with the studies reporting that fields receiving manure are the largest sources of N_2O emissions from manure (e.g., Chadwick et al., 1999). However, the fields were simulated as the largest source of the N_2O emissions under S4 with 50% of the solid manure applied into the fields. This result suggests the importance of manure fate on the N_2O emissions from different components in a dairy farm. It should be noted that these results are only for one dairy with specific conditions and assumptions that may be different from conditions in other studies. Therefore, the differences between the simulations and other reports do not mean one method is outperforming another.

Table 14. Simulated annual total CO_2, CH_4, N_2O, and NH_3 emissions from different components within the target farm

	CO_2 emission ($MT\ C\ yr^{-1}$)	CH_4 emission ($MT\ C\ yr^{-1}$)	N_2O emission ($MT\ N\ yr^{-1}$)	NH_3 emission ($MT\ N\ yr^{-1}$)
Baseline				
Housing	6073.7	657.7	8.6	50.3
Solid pile	336.9	0.0	1.4	53.6
Lagoon	186.6	177.1	0.7	62.6
Field	589.0	0.0	3.3	38.4
Housing manure removal by water flushing				
Housing	6074.5	665.1	4.2	50.2
Solid pile	652.7	0.6	0.8	73.6
Lagoon	184.0	174.4	0.3	65.4
Field	590.6	0.0	3.4	38.5
50% of housing solid manure was transferred into lagoons				
Housing	6073.7	657.7	8.6	50.3
Solid pile	398.8	0.1	1.4	57.2
Lagoon	293.7	281.7	0.7	71.5
Field	707.6	0.0	4.0	44.2
All housing manure was transferred into lagoons				
Housing	6073.7	657.7	8.6	50.3

Solid pile	None	None	None	None
Lagoon	527.9	508.9	0.9	102.8
Field	999.8	0.0	6.6	67.6
50% of solid manure piles were applied into fields				
Housing	6073.7	657.7	8.6	50.3
Solid pile	325.7	0.0	1.4	52.5
Lagoon	186.6	177.1	0.7	62.6
Field	2091.0	0.0	10.3	56.5

Technology Transfer of CADEM To CARB

To request the CADEM system, please contact Dr. Seyedmorteza Amini at:

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To facilitate the model application in California dairies, the following activities and materials have been conducted or delivered through this project:

- New model interfaces (Figures A1 to A7) have been developed to support the new incorporated processes and equations and the new developed functions
- Model user's guide has been updated to describe the new incorporated processes and equations and the new developed functions, and has been delivered to CARB along with this final report
- An example of CADEM input file for conducting whole farm simulation has been delivered to CARB
- Discussions and meetings have been held to introduce model input parameters and output variables

- Discussions and meetings have been held to ask feedbacks from CARB staff and add additional features for the model interface based on the feedbacks to ensure the tool meets the needs of CARB staff and stakeholders.
- Discussions and meetings have been held on converting annual dairy report and waste management plan to CADEM requested parameters
- A model training has been held to further introduce the CADEM system and clarify questions/concerns from CARB staff

Limitations

There are several limitations in this study. First, CADEM has not been evaluated against GHG and N gas fluxes from manure storage areas in California dairies due to limited field data that are proper for evaluating the model. In order to evaluate simulations of GHG and N gas fluxes from manure storage areas, it is ideal to have high frequent observations of GHG and N gas fluxes during different seasons, annual total emissions, as well as relevant model input parameters (e.g., climate, structure and characteristics of manure storage areas, manure transfers among farm components, and manure management), which are not available at this stage. Second, not all the model input parameters (e.g., feeding information, manure distributions among different storage areas) are available to conduct farm-scale simulations, and some assumptions have been made for conducting the simulations. Therefore, the farm-scale simulations are subject to uncertainties and limitations in model input parameters. Third, CADEM has incorporated processes to simulate effects of two types of feed additives on mitigating enteric CH_4 flux from dairy cattle. However, potential effects of the feed additives on manure (amount and properties) and GHG and N-gas from manure management have not been characterized and simulated. Further studies need to be performed to further evaluate the model against field data, develop database of model input parameters, and improve model representation of dairy activities that affect C, N, and P dynamics in dairy farms in California.

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Appendix A

Appendix: Newly developed interfaces in CADEM

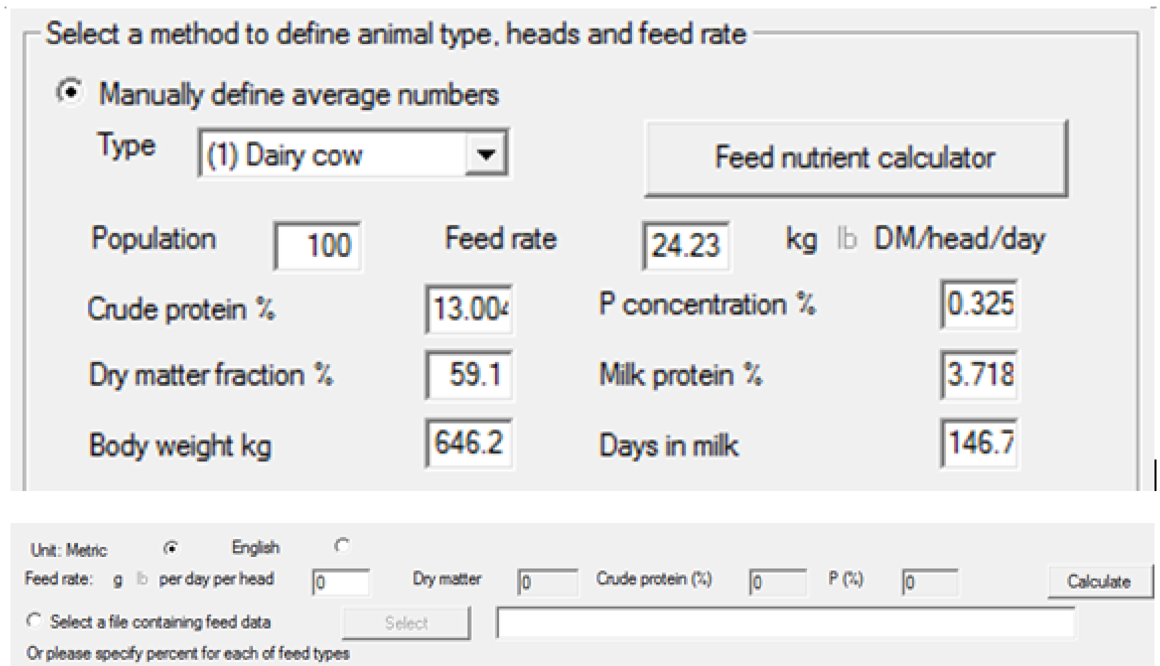

Figure A1. Model interfaces for receiving new input parameters to calculate GHG flux and manure excretion from dairy cattle.

Figure A2. Model interface for selecting method to calculate GHG flux and manure excretion from dairy cattle and receiving parameters to calculate mitigation of CH_4 flux by feed additive.

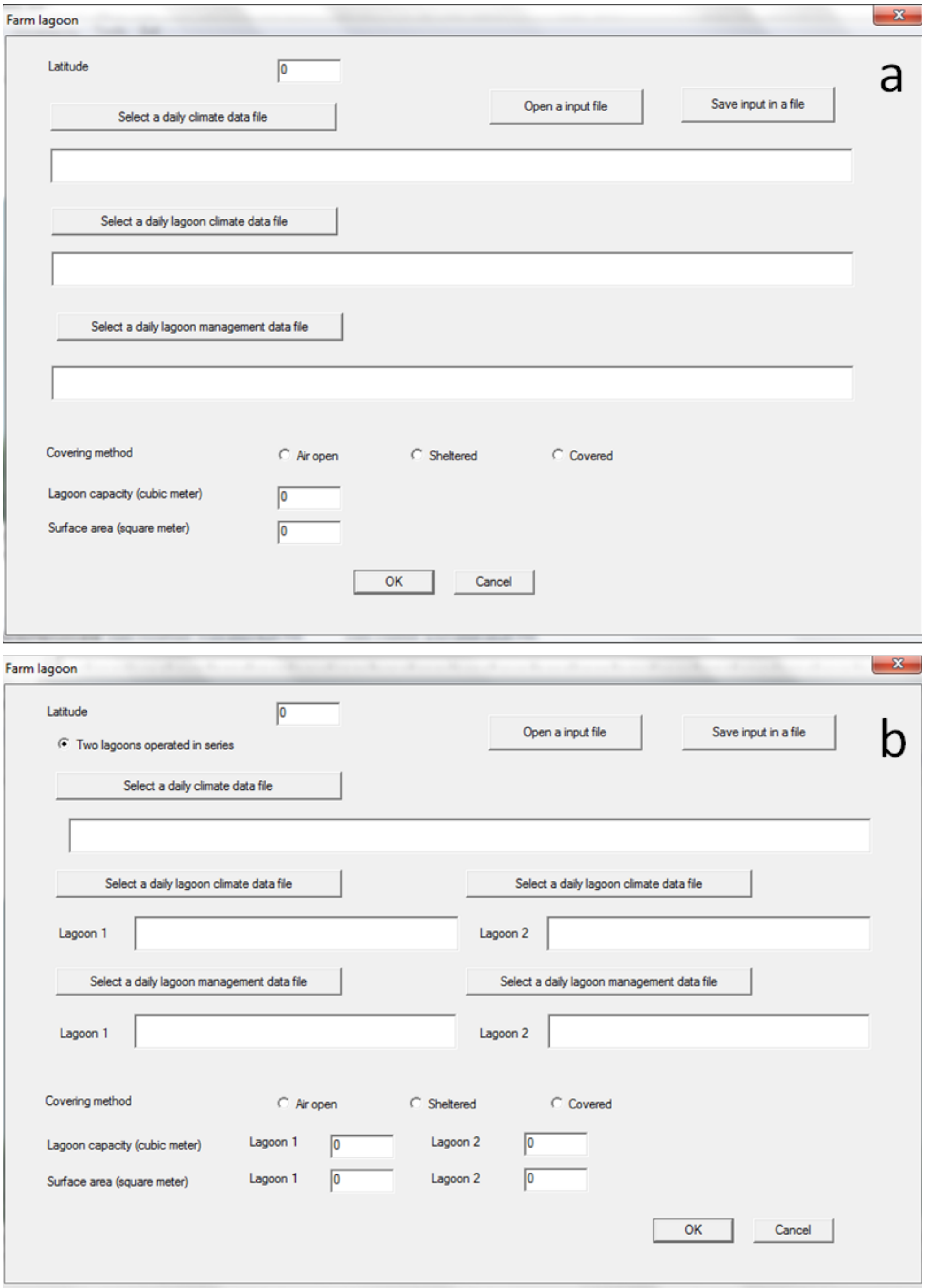

Figure A3. Old (a) and new (b) interfaces for simulating water, C, N, and P dynamics in slurry manure storage areas.

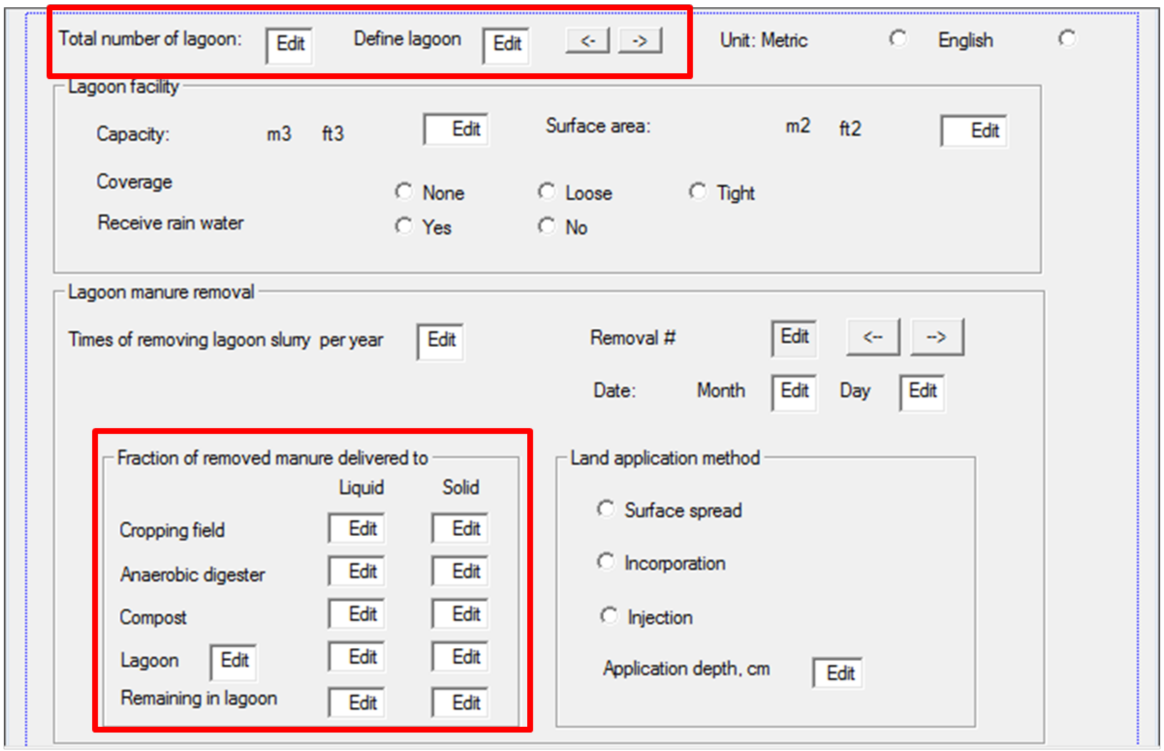

Figure A4. New model interface for setting input parameters (e.g., properties and manure management practices) of different slurry storage areas. The updated interface has been marked using red rectangles.

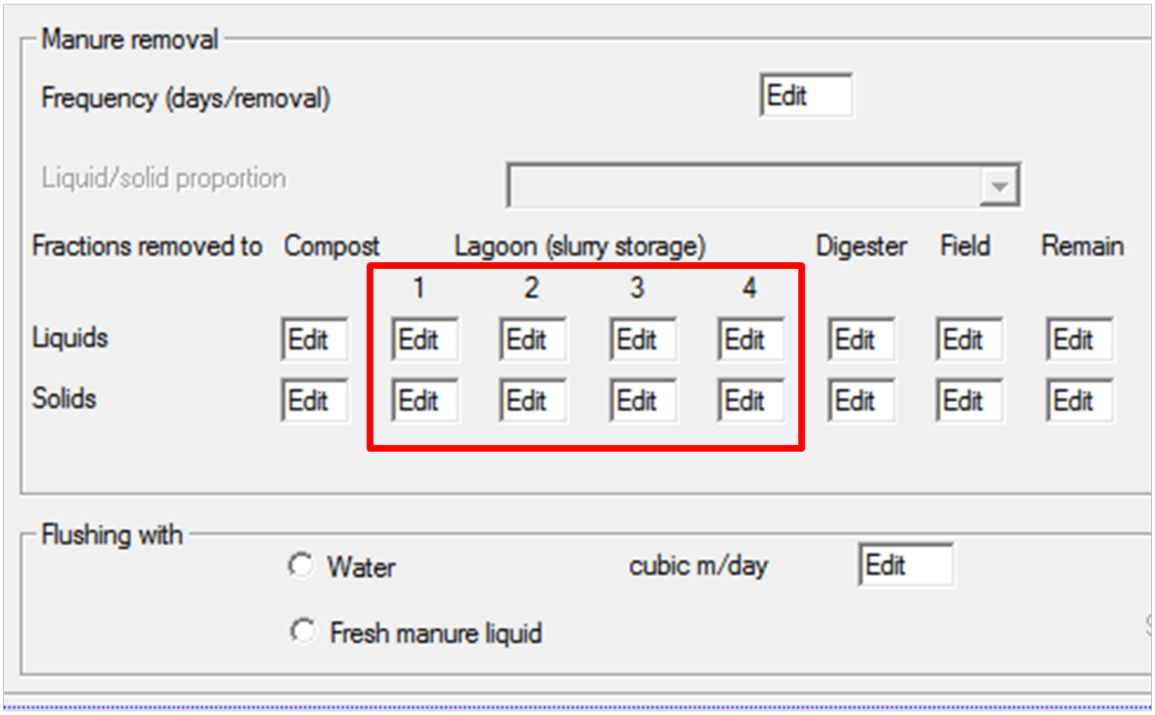

Figure A5. New model interface for simulating manure removal from housing to different slurry manure storage areas. The new model interface allows users to set manure transfers from housing to multiple lagoons. The updated interface has been marked using a red rectangle.

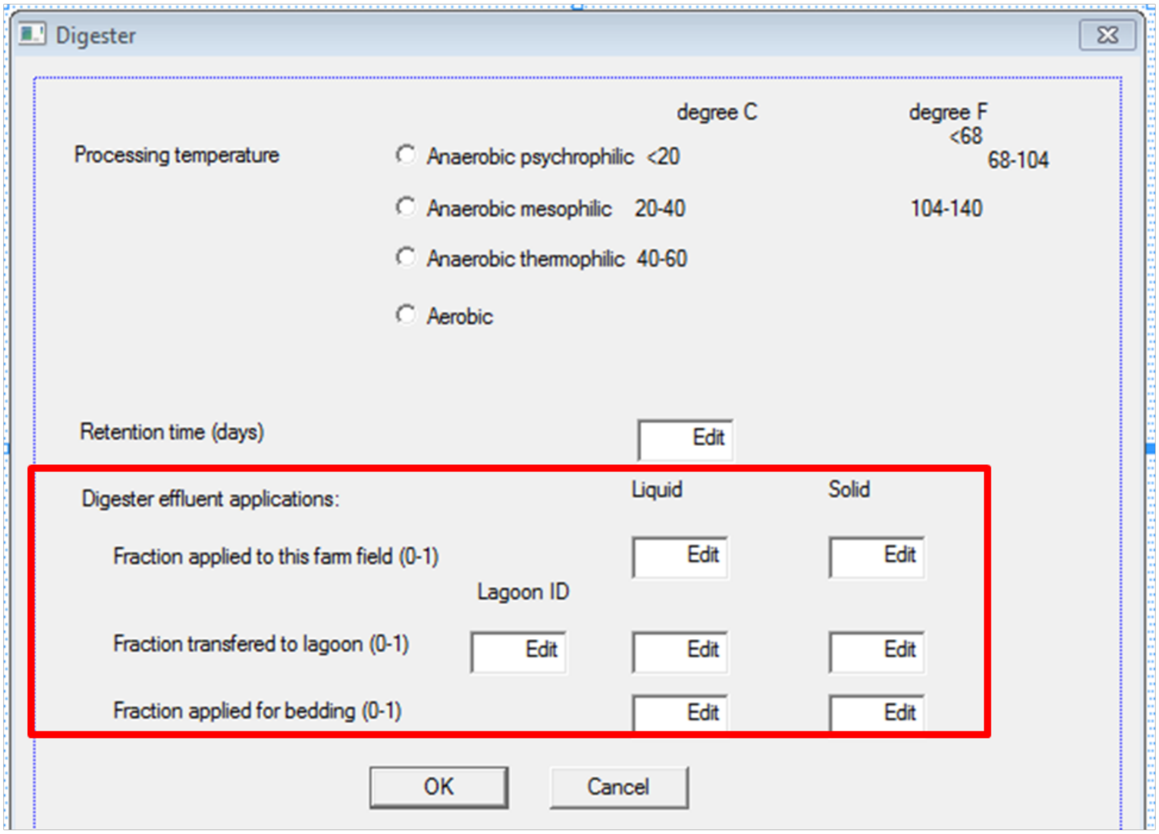

Figure A6. New model interface for simulating manure transfers from digester to slurry manure storage areas. The new model interface allows users to set manure transfers from digester to multiple lagoons. The updated interface has been marked using a red rectangle.

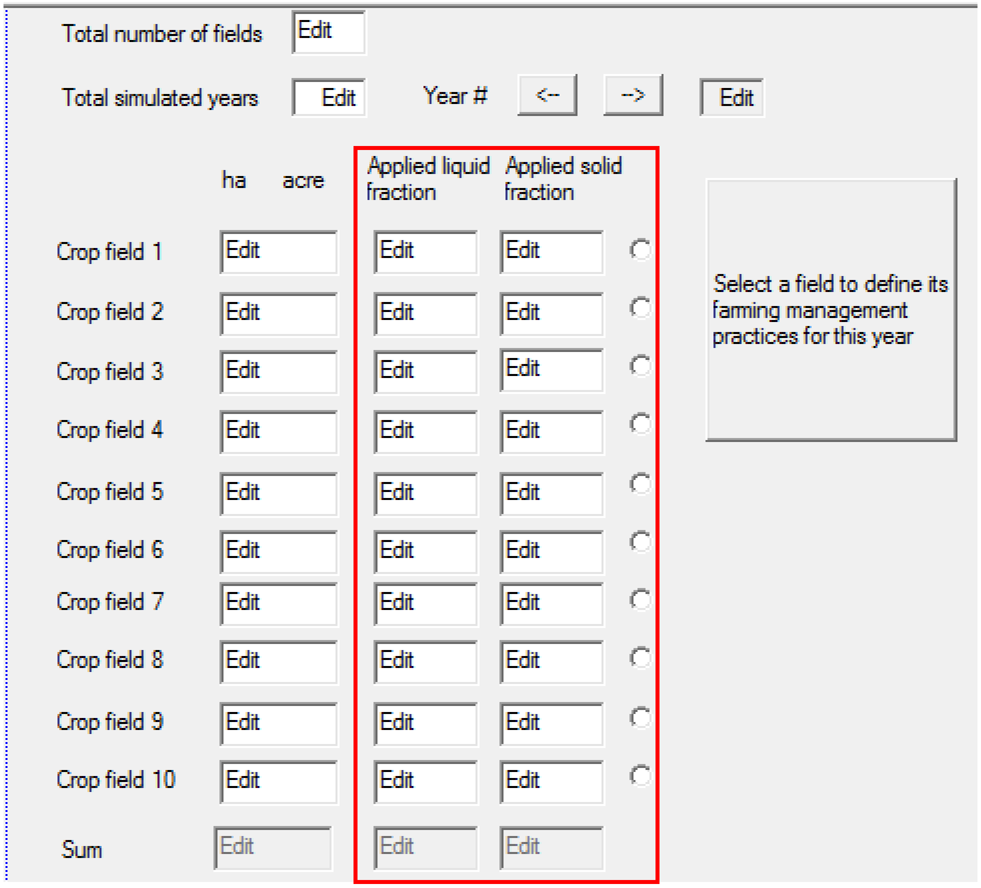

Figure A7. New model interface for simulating manure amendments from housing and/or storage areas to fields. The new model interface allows users to distinguish solid and liquid fractions of manure. The updated interface has been marked using a red rectangle.