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Dairy-CropSyst: Gaseous emissions and nutrient fate modeling tool

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ABSTRACT

Dairy concentrated animal feeding operations (CAFO) are required to implement nutrient management plans enforced by environmental protection agencies to minimizing the risk of water resource degradation and to report gaseous emissions when they exceed certain threshold values. Although tools exist to aid in completing such tasks, few of the tools integrate the impact of on-farm manure treatment unit operations such as anaerobic digestion, solids separation, and nutrient recovery. Furthermore, existing tools do not estimate the nutrient value of recovered products and effluent leaving the dairy system or the nutrient fate after effluent is applied to crop fields.

Dairy-CropSyst is a decision support tool for researchers and CAFO managers aimed at evaluating the effects of different manure treatment unit operations on gaseous emission and nutrient fate in dairy systems. The model tracks nutrients through the dairy system, including inorganic and organic forms of carbon, nitrogen, and phosphorus. This is accomplished by integrating established transformation and emission equations, performance parameters of manure treatments from industrial data and literature, and using a cropping system model for the land application evaluation. Comparison of simulated values with observed emissions indicated that model performance was reasonable. The overall correlation coefficient of observed and predicted ammonia and methane emission from dairy manure management was 0.72 and 0.58 respectively. Simulated and observed N_2O emission were found in close agreement before and after the irrigation event, however, the model over estimated N_2O emission after irrigation events (Coefficient of Residual Mass = −0.87). The use of Dairy-CropSyst has the potential to assist the dairy industry in decision making on manure management treatment strategies and as a tool for reporting GHG and ammonia emissions.

1. Introduction

Due to population growth, global food demand is increasing rapidly, as are the environmental impacts of agricultural expansion (Alexandratos and Bruinsma, 2012). The reduction of gaseous emission and nutrient losses while meeting food needs has become an international policy issue (UN-FCCC, 2011). Agriculture is a source of three primary greenhouse gases (GHG), methane (CH_4), carbon dioxide (CO_2) and nitrous oxide (N_2O) and is responsible for 24% of global GHG emissions (IPCC, 2014). Livestock operations are a major source of these emissions and are of particular concern when many animals are confined in a small area. Globally, dairy operations are responsible for 4% of net anthropogenic GHG emissions (Gerber et al, 2010). In the United States, over the past three decades the CH_4 and N_2O emissions from dairy manure management increased by 115% and 11%, respectively (USEPA, 2015). It is also estimated that more than 80% of NH_3 emissions are related to agricultural operations, with a major portion coming from livestock operations (NOAA, 2000). Dairies contribute more than 20% of the total NH_3 emissions (Sakirkin, 2011), where the estimated loss of ammonia as a percentage of nitrogen (N) in manure is about 38% (USEPA, 2004). Excess soil nutrient in associated dairy farmland is another challenge to these large dairy operations. Bulk amounts of manure produced on these facilities are usually applied to nearby fields due to associated cost if hauled to distant locations

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(Heathwaite et al., 2000). As a result, manure-derived nutrients are often in surplus relative to the available agricultural land (USDA, 2001) and may significantly impact water quality, land, and biodiversity if not managed properly (USEPA, 2012; Steinfeld et al, 2006). As in North America, the European Union agro-environmental projects also aim to reduce the environmental impact of intensive dairy operations (Casey and Holden, 2005; Gibon, 2005), particularly gaseous emissions (Saggar et al., 2004) and nitrates in groundwater which were above acceptable levels (25 mg/l) on 85% of EU farmland (EC, 2000). Similar concerns regarding intensive dairy operations exist in Asia (Fanet al., 2017; Gao et al., 2014; Zhu et al., 2014).

In the United States, the concentrated animal feeding operations (CAFOs) are required to develop and implement a farm-specific Comprehensive Nutrient Management Plan to minimize water pollution from livestock manure (USDA and USEPA, 1999). CAFOs are required to report NH_3 emission if they exceed 45 kg NH_3 per day (USEPA, 2010). Under the Kyoto Protocol, European countries are committed to reduce GHG emission where a majority of the anthropogenic emission is from livestock operations (Beukes et al., 2010), while under the Clean Stream Accord, dairies with high stocking densities must implement best management practices to protect water resources (MfE, 2003). Toward these ends, the use of emission factors has proven insufficient for quantifying emissions due to the high variability in ambient environmental conditions and feed composition (NRC, 2003). The variability in gaseous emission from barn, lagoon storage, and field applications of manure is mainly caused by environmental factors, soil properties and agricultural practices (Saggar et al., 2004). Compared to model simulation and emission factors, direct measurements are relatively accurate, but they are time consuming and expensive. Therefore, the NRC (2003) recommends an integrated modeling approach to estimate gaseous emissions and to monitor nutrient fate from a whole-farm perspective (Crosson et al., 2011).

The use of modeling as a dairy CAFO decision support tool is beneficial due to the complexity of processes, management strategies and environmental factors (Cabrera et al., 2005). A detailed review of models for dairies is provided by Crosson et al. (2011). Models such as FARMMIN (Van Evert et al., 2003), FarmGHG (Olesen et al., 2006), DairyWise (Schils et al., 2007), HOLOS (Little et al., 2008), OVERSEER (Wheeler et al., 2008), $SIMS_{DAIRY}$ (Del Prado et al., 2011), NTT (Saleh et al., 2011), Manure-DNDC (Li et al., 2012), and IFSM (Rotz et al., 2012) are designed to predict gaseous emission from livestock manure handling systems. However, these modeling tools consider only the traditional manure management strategies and do not consider the effect of emerging manure treatments for nutrient recovery. In order to comply with environmental regulations, various techniques are available for manure treatments to reduce emissions and to avoid nutrient overloading on dairy lands. These treatments not only reduce nutrient concentrations in effluent, but they also affect the partitioning between organic and inorganic constituents of the effluent (Frear and Ma, 2015). Knowledge of the impact of manure treatments is necessary for planning and optimizing the efficiencies of manure management systems, nutrient fate, and gaseous emissions. Modeling tools will not effectively predict nutrient fate and gaseous emissions if they do not consider the effects of manure treatments (Khalil et al., 2016). Dairy-CropSyst is a recent addition specifically designed to track nutrient fate and gaseous emission from dairy CAFOs with liquid manure handling systems. It has the advantage of considering the effect of existing and emerging manure treatment options, including coarse fiber separation, anaerobic digestion (AD), fine solids removal, and ammonia recovery to traditional manure management. Different research studies (Amon et al., 2006; Schils et al. 2005) have pointed out the importance of integrated assessment of the whole cycle if the objective is to recommend a mitigation technique. If the whole cycle is not assessed, it is likely that the recommended control or technique would reduce losses at one stage, but increase losses at a later stage in the life cycle. With Dairy-CropSyst, the manure treatment options can be arranged in a certain sequential order from barn to cropland, and permit treatment evaluation for a dairy manure complete farm cycle perspective.

This paper describes Dairy-CropSyst and evaluates its performance by comparing model simulations to observed emissions from dairy CAFOs including NH_3, CH_4, and N_2O from various dairy farm unit operations. An analysis was also conducted to illustrate the impact of farm manure management alternatives on model predictions.

2. Model description

Dairy-CropSyst is a decision support tool for CAFO managers, extension specialists, and researchers to evaluate the effects of diverse manure treatment strategies on net GHG emissions and manure nutrient fate through the dairy system, from barn to application of manure in the field. This is accomplished by integrating established models dealing with manure production and associated emission during manure management, performance parameters of different manure treatments from industry data, and using the cropping systems model, CropSyst. On a dairy facility during handling, storage, and after field application the manure constituents undergo biochemical changes driven by environmental factors, particularly temperature and wind speed, and physiochemical properties of the manure, such as pH. Within the model and at a daily time step, mass balance of emissions and manure-derived nutrients, in organic and inorganic form, resulting from biochemical changes that occur across the barn to field is maintained through specific treatment steps, and then transferred from one unit operation to another. Fig. 1 shows available scenarios for manure treatment options and their resulting nutrient production and emissions. The model interface allows the user to create a simulated dairy farm by entering the dairy farm configurations and management information, as well as crop, soil, weather, and manure treatment options. The essential input parameters required to generate a simulation scenario are listed in Table 1.

2.1. Dairy Sub-Model

The dairy component deals with manure production and its lifecycle on the dairy facility. It has animal, barn, and lagoon components and deals with manure production, handling and storage. Flow of manure carbon (C), nitrogen (N), and phosphorous (P) in organic, inorganic, and gaseous form is tracked using empirical and process based models. A description of these models is provided in Appendix A.

2.1.1. Animal component

The animal component estimates the amount of manure produced, its nutrient composition, and direct GHG emissions on a single lactating cow basis. The total manure, urine volume, and dry matter content in excreta is determined as a function of milk production, animal body weight, and dry matter intake in feed using empirical equations derived from data sets collected on dairy herds at Ohio State University, University of California, Pennsylvania State University, and Washington State University (Nennich et al., 2005). The amount of N and P in manure is estimated using the American Society of Agricultural and Biological Engineers (ASABE) Standard (Standard D384.2: Manure Production and Characteristics; ASABE, 2005), while the C content is determined from the C to N ratio of fresh manure. The animal component keeps separate accounts of organic and inorganic N excreted in manure. Urine N is derived from a wide range of dairy feed composition (Bannink et al., 1999) with the major fraction of urine N in the urea form and estimated using a relationship developed by de Boer et al. (2002). The major fraction of the N in feces is in an organic form and contains a very small fraction (about 5%) of inorganic N in ammoniacal form (Van Horn et al., 1994). The model calculates organic N from mass difference between total N and inorganic N found in both the urine and feces fractions of manure.

Dairy animals contribute a large portion of the GHG emissions

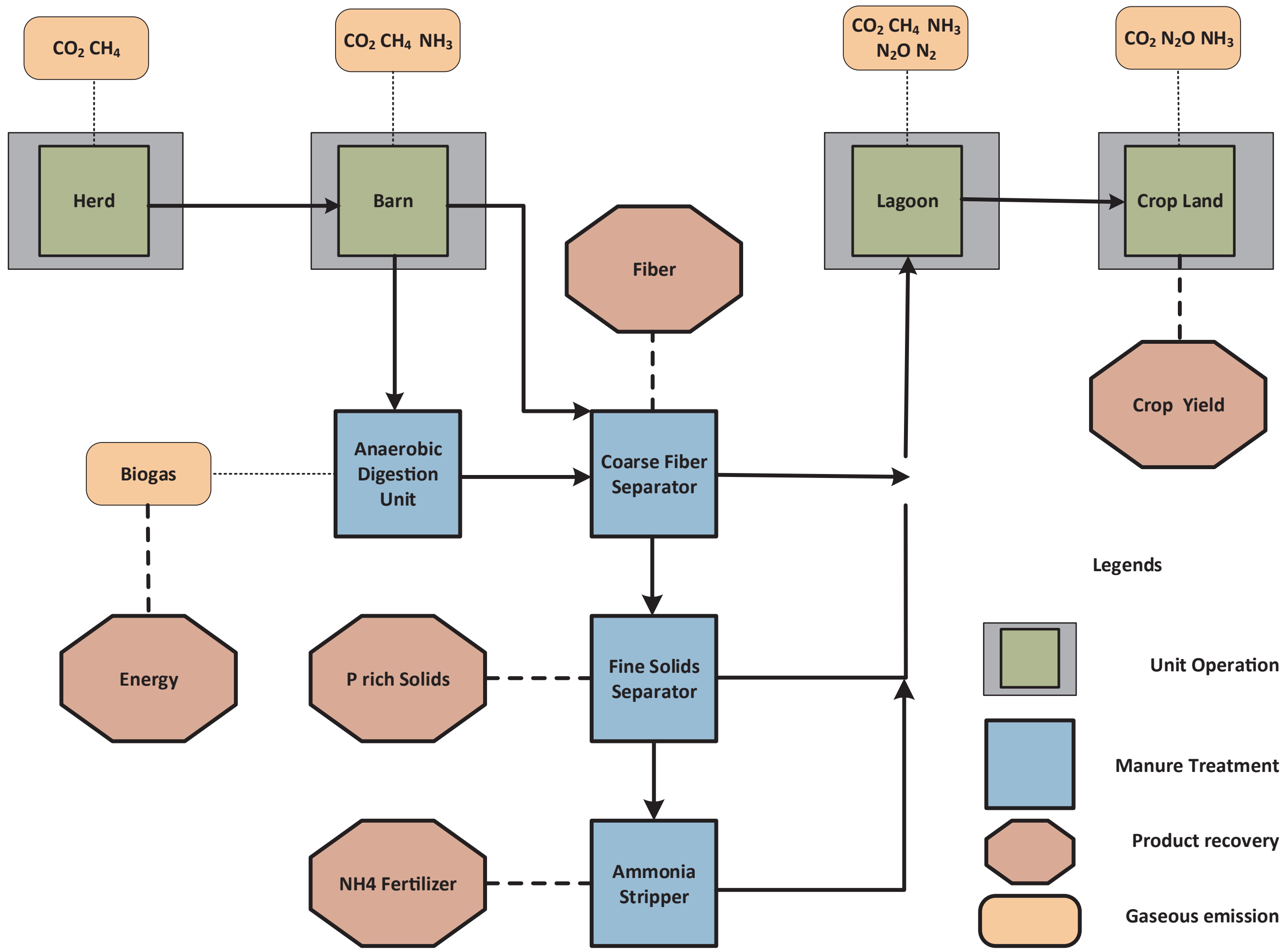

Fig. 1. Schematic representation of manure flow, gaseous emissions, and value-added product recovery for dairy manure from barn to cropland application. The possible manure flow paths are represented by solid lines, gaseous emissions are represented by dotted lines, and product recovery is represented by dashed lines.

emanating from a dairy CAFO. Main GHG emitting directly emitted from the dairy cow is CO_2 and CH_4 through respiration and enteric fermentation. As per IPCC, 2006 Guidelines, the CO_2 emissions from animal respiration are not quantified and annual net CO_2 emissions are zero. This is due to the fact that CO_2 up taken by plants for photosynthesis is consumed by animals as feed and then emitted through respiration back to the atmosphere. However, for Carbon mass balance the model keeps track of both CO_2 and CH_4 emitted directly by the animal. The CO_2 emission from animal respiration is estimated as a function of dry matter intake in feed and dairy cow body weight using a model proposed by Kirchgessner et al. (1991), while CH_4 emission from enteric fermentation is based on the approach of Rotz and Chianese (2009). Direct emissions of N_2O and NH_3 from dairy animals are negligible (IPCC, 2006; Jungbluth et al, 2001), therefore the model does not consider direct emissions of these gases from the herd.

2.1.2. Barn component

Fresh manure is deposited on the barn floor assuming a uniform distribution and equal quantity of manure dropping between urination events. The main processes occurring on the barn floor are urine urea hydrolysis and subsequent NH_3 volatilization. Urine urea is hydrolyzed to NH_3 rapidly when it comes in contact with urease present in the fecal part of the manure. In Dairy-CropSyst the urea hydrolysis process is modeled using the Michaelis Menten equation, where the rate of NH_3 formation is limited by substrate (urea) concentration in manure and is in gaseous and aqueous equilibrium depending on the manure slurry temperature and pH (Ni, 1999). The model estimates NH_3 volatilization from the dairy barn alley using a mechanistic approach (Monteny et al., 1998). The NH_3 volatilization from the barn floor is directly related to the total ammoniacal Nitrogen (TAN) present in the manure, NH_3 fraction, portioning of NH_3 between gaseous and liquid forms, and the convective rate transfer it moves into the atmosphere. The fraction of the ammonia (f) in TAN is dependent on the slurry pH, temperature, and acid dissociation constant (K_a). Diary-CropSyst is using value for K_a of 8.11×10^{-11} for dairy manure as reported by Monteny et al. (1998). Further partitioning of NH_3 between liquid and gas phase is dependent on manure slurry temperature and predicted using Henry's constant (H). The NH_3 eventually volatilizes from the barn floor to the surrounding atmosphere at the rate modeled by mass transfer coefficient (k) depending the surface roughness and wind speed (ws) at the barn floor level. The governing equation for k, f, and H is provided in Appendix A. Due to rapid hydrolysis of urine urea the NH_3 volatilization at the barn is simulated at a 1-minute time step and is integrated over a 24 hr period.

Fresh manure deposited onto the barn floor may release a small fraction of GHG (Kaharabata et al., 2000) due to manure microbial activities initiated in the rumen under anaerobic conditions. Carbonaceous emissions are modeled using empirical models with air temperature and barn alley area as input parameters, while for N_2O the model uses an emission factor of 2×10^{-5} kg N_2O-N m^{-2} d^{-1} (Rotz and Chianese, 2009). The manure is scrapped from the barn floor periodically and flushed out with water from the milking parlors. For manure mass balance the model assumes a typical water application rate of 64 L cow^{-1} d^{-1} (Frear and Ma, 2015).

Table 1
Essential model input parameters. Based on these parameters related to feed characteristics, farm management practices, and environmental drivers, Dairy-CropSyst estimates gaseous emission, value-added product recovery, crop biomass production, carbon footprint, and soil nutrient balance.

Input/Parameter	Description	Units
Lot	Number of animals	Cow
BW	Body weight	kg
DMI	Dry matter intake	kg d^{-1} cow^{-1}
Diet CP	Diet crude protein	%
MP	Milk production	kg d^{-1} cow^{-1}
Me	Metabolic energy in diet	MJ cow^{-1} d^{-1}
Starch_f	Diet starch fraction	–
ADF_f	Diet acid detergent fiber fraction	–
pH	Manure pH	–
Barn floor	Barn alley area	m^2
Nos of barn cleaning	Flush/Scrape frequency	d^{-1}
Lagoon area	Lagoon surface area	m^2
Max Vol	Maximum manure holding capacity of lagoon	m^3
Manure treatments	Type of manure treatments and their sequential order	–
Lagoon management	Irrigation timing, frequency, amount	–
Weather data	Ambient and barn weather data	–
Soil	Soil texture, depth, and initial soil nutrients	–
Crop	Crop phenology - sowing, emergence, flowering, maturity	–
Crop management	Irrigation amount and frequency, fertigation and bio-matter application, tillage and crop rotation	–

2.1.3. Lagoon component

On dairy CAFOs the manure is stored in a lagoon until field conditions allow manure application. In Dairy-CropSyst the lagoon component is parameterized by its total capacity and is directly related to the herd size, surface area, barn effluent, and manure land application frequencies. The input flow includes the daily multiple scrapes from barn and milking parlors with or without manure treatments and direct precipitation on lagoon surface, while the out flow includes seepage, evaporation, and volumes applied to cropland. Evaporation and seepage from the dairy lagoon is estimated using a relationship developed by Ham (2002). The main processes modeled in the lagoon are the decomposition of organic matter causing emission of CH_4 and CO_2, ammonification associated with organic N mineralization, nitrification and denitrification and associated N_2O emission, and NH_3 volatilization driven by biophysical factors. The NH_3 volatilization from the lagoon follows the similar process as in the barn, the only difference being the wind speed considered to calculate the mass transfer coefficient. In weather file the wind speed measurements are generally taken a couple of meters above the lagoon surface, for NH_3 volatilization the wind speed need to be adjusted to obtain value at lagoon surface. The adapted equation to adjust wind profile over the lagoon surface is provided Appendix A Lagoon NH_3 emission. The lagoon mass balance and associated biochemical processes are elaborated in Fig. 2.

Decomposition of organic matter is modeled using a three-pool, first order decay reaction (Paul et al., 1999) at a daily time step. The total C concentration and its biochemical composition vary if the manure is treated, hence the first-order decomposition rate. Therefore, manure-specific decomposition rate constants (Khalil et al, 2016) were used for labile- and slow-decomposing C pools if the manure is undergoing treatment, while for the recalcitrant C pool the decomposition rate content was set to 2.74×10^{-6} d^{-1} (Paul et al., 2001). Fast cycling, slow, and recalcitrant C pools are estimated in manure assuming that the fast cycling labile C pool is composed of volatile fatty acids (VFA), lipids, and readily decomposable carbohydrates, whereas non degradable carbohydrates make up the slow C pool, and lignin is added to the recalcitrant pool (Frear and Ma, 2015).

The decomposition function uses ambient daily average temperature for modeling the temperature effect on the decomposition of organic manure in the lagoon. This model assumption is based on the work of Pratt (2013) who found an overall similarity between ambient and shallow lake water temperature. The lag time between peak air and water temperature varied up to 3 h, though the fluctuations of temperature in water bodies is less extreme due to the high heat capacity of water compared to gaseous media (Kalff, 2002). Manure organic matter decomposition rate constants determined empirically in laboratory at 25 °C under anaerobic conditions are adjusted for daily ambient temperature using a factor developed by Schomberg et al. (2002). Though dairy lagoons are considered to be anaerobic due to high solids loading and depth, wind-driven surficial oxygen transfer allows a shallow aerobic layer to exist (Ro and Hunt, 2006). The lagoon C mineralization rate is adjusted for variation in dissolved oxygen using correction factors developed by Asaeda et al. (2000).

The C mineralized during decomposition is released as CO_2 and CH_4. In the shallow aerobic overlying surface layer, the C is mineralized in the form of CO_2, while in the anaerobic layer 60% of the decomposed organic C is released as CH_4 and 40% as CO_2 (Van Horn et al., 1994). The CH_4 produced in the lagoon is released to the atmosphere due to its low solubility, however part of the CO_2 is dissolved in lagoon water and is modeled as a function of lagoon water temperature (Carroll et al., 1991). During decomposition organic N is converted into an inorganic form. This ammonification is computed using a manure organic C:N ratio and is added to the lagoon ammoniacal N (TAN) pool. A number of studies (Rumberg et al., 2008; Neger, 2002) attribute N losses from the lagoons to NH_3 volatilization, although other studies also find N losses in the form of N_2 and N_2O from manure storage (Hensen et al., 2006; Harper et al., 2000). In dairy lagoons, due to prevailing anaerobic conditions, nitrate formation is very low and is only likely to happen in the upper shallow aerobic layer if no aerator is used. The nitrification processes in the lagoon are modeled using Monod's kinetics where TAN concentration and dissolved oxygen are limiting factors, and the process is corrected for temperature and pH (Kadlec and Knight, 1996). Nitrates produced are reduced to nitrites and eventually to N gas (N_2) and N_2O by denitrifying bacteria. Denitrification in the lagoon is modeled as first order kinetics using the Arrhenius equation to account for the temperature effects (Kadlec and Knight, 1996). The partitioning ratio between N_2 and N_2O is modeled after Parton et al. (1996) considering only nitrate availability as a limiting factor in the lagoon.

2.2. Nutrient management add-ons

Dairy-CropSyst allows the manure flow routing to different treatments in a sequential order. The model calculates the value-added products recovered from manure during treatment as well as manure effluent with altered nutrient constituents after treatment. The model allows the user to select manure treatment options including anaerobic digestion, coarse fiber separation, fine solids removal, and ammoniacal N recovery while building a particular dairy CAFO scenario. Solids and nutrient recovery factors for different treatments are based on published values and industry data. A summary of manure mass balance when subjected to different treatments is provided in Appendix B.

2.2.1. Anaerobic Digester

The use of AD as a means to reduce GHG emissions and as a source of alternative energy from manure is gaining popularity in the United States. An AD plant is an engineered facility optimized for anaerobic decomposition of manure to produce biogas for energy production and reduction of downstream solids flow to lagoon storage which minimizes CH_4 emission. Manure flowing into the AD is the total manure excreted by the dairy animal plus the milking parlor waste water which is typically equivalent to the volume of manure produced (Frear and Ma, 2015). In Dairy-CropSyst an AD manure treatment is modeled using

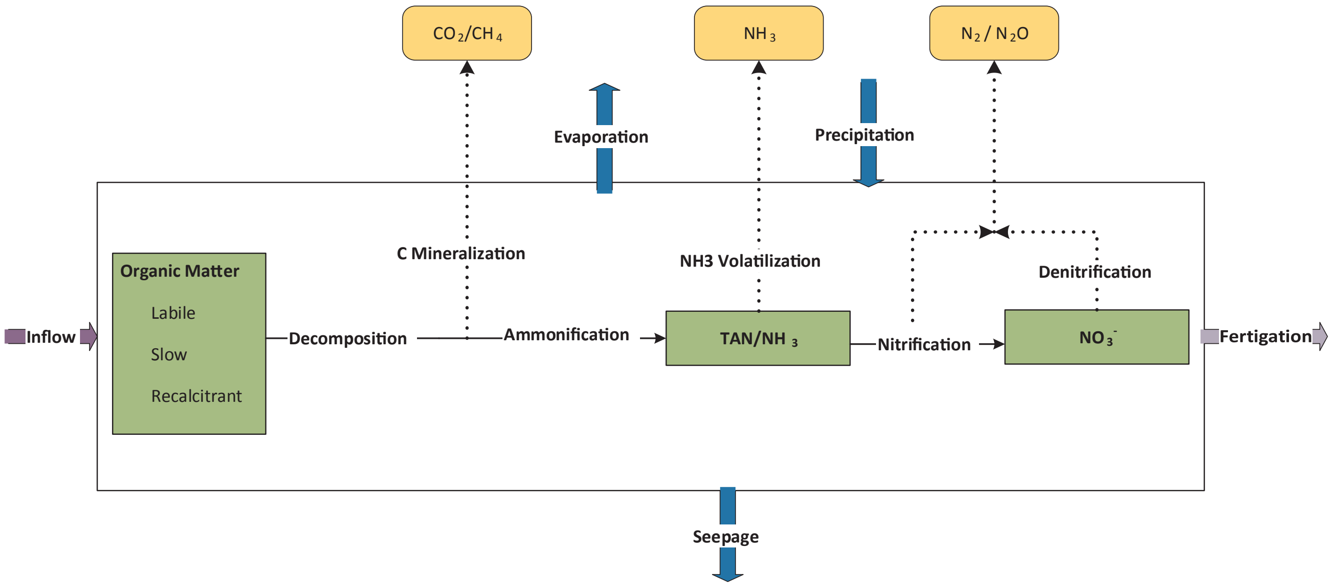

Fig. 2. Lagoon mass balance and major biochemical processes occurring in dairy lagoon. Processes representing gaseous emissions are represented by dashed lines while chemical transformation are represented by solid lines.

reduction factors to parameterize manure effluent, and calculates the biogas produced at a daily time step. The AD model is characterized by its ability to reduce total solids (TS), volatile solids (VS), and total C (TC) by a consortium of microbes under anaerobic conditions for a particular hydraulic retention time (HRT). Literature and various industry reports indicate a VS reduction of about 35–45% for 20–30 days of HRT when operated under mesophilic conditions (35–38 °C) (Demirer and Chen, 2004; Karim et al., 2005; US-EPA, 2004; US-EPA, 2005). Default model parameters for TS and VS reductions are set to 30 and 42% respectively, TAN increase is set to 25%, and TC is reduced by 40% (US-EPA, 2005; Frear and Ma, 2015). No change to total Kjeldahl N (TKN), total N (TN), and total P (TP) is assumed during manure AD treatment. The AD treatment reduces the labile and slow C pool by 53 and 30%, respectively, while no changes are made in the recalcitrant C pool (Frear and Ma, 2015). The model assumes that 52% of the C recovered by AD is mineralized into CH_4, while the remaining carbon is mineralized to CO_2. Different commercial models including continuous flow, complete mixed, and covered lagoon type plants are used in practice. Model default values are based on industry data and may differ from one AD plant to another depending on the type of AD, substrate composition, and prevailing biophysical conditions inside the plant. The use of site specific reduction factors is therefore recommended.

2.2.2. Solids separation

Solid-liquid separation not only removes nutrient-rich solids from manure but also offers the benefit of reducing bulk volume and solid loading into the lagoon, resulting in reduced gaseous emissions (Møller et al., 2000). The separated liquid stream is also easier to handle during field application due to lower concentration of solids and reduced particle size and thus can be applied through irrigation systems without clogging pipes and sprinkler nozzles. Solid separation also tends to reduce the odor emission from lagoon and the recovered solids have nutrient value which can be transported off the farm. Dairy-CropSyst simulates the effect of both coarse fiber removal through screen separations and/or settling basin, and fine solid removal through dissolved air floatation (DAF) or centrifugation. The characteristics and operational efficiency of a particular solid separation technique are reflected in their ability to reduce TS, VS, TAN, TKN, organic N, TP, and volume reduction of manure effluent after treatment. Dairy-CropSyst reduces TS, VS, TKN, organic N, and TP by factors of 40, 50, 12, 10, and 8%, respectively, when manure is treated for coarse fiber removal. These constituents are further reduced by 59, 49, 33, 69, and 80%, respectively when coarse fiber removed effluent is further treated for fine solids removal (Frear et al., 2006; Frear, 2012; Frear et al., 2015; Frear and Ma, 2015).

Coarse fiber separation is effective for removing lignin from manure, thereby reducing the recalcitrant C pools by 75%. The recalcitrant pool is further reduced by 78% when effluent is treated for fine solids removal through DAF. Phosphorous is a high value nutrient in dairy manure and is generally found in excess of crop need in most of the crop lands receiving excessive manure applications. Fine solids removal is more effective in recovering manure P (80% recovery) than other treatments (Frear and Ma, 2015).

2.2.3. Ammoniacal N recovery

High N losses from manure in the form of NH_3 volatilization create air quality problems. Particulate matter ($PM_{2.5}$) forms when the NH_3 reacts with impurities present in environment, and excess N leaching to water resources causes waterborne diseases in humans. The emitted NH_3 deposition around feedlots is a significant (Shen et al., 2016) and may impact the ecosystems of the surrounding and surface water quality. Potential economic benefits accrue from N recovery as source of fertilizer. All of these factors argue for dairy CAFOs to recover the ammoniacal N from manure. The NH_3 volatilization is further triggered when the manure is undergoing treatment for biogas production as AD increases both the TAN and the pH of effluent or digested manure (Koirala et al., 2013) thus increasing the risk of ammonia volatilization from lagoon storage. Ammonia stripping is a widely used technique for TAN recovery from wastewater. This stripping is usually performed at a pH of 10.5 to 11.5 and at high temperature with the high-alkaline effluent pH brought back to near initial pH before storage in the lagoon. Ammonia stripping can be an eco-friendly and economical process, particularly when co-digestion is carried out in the AD (Astill and Shumway, 2016). Dairy-CropSyst assumes that 70% of TAN is recovered from manure when treated for TAN recovery (Zhao et al., 2015).

2.3. Field application component (CropSyst)

Field application of manure is simulated by CropSyst (Stöckle et al., 1994; Stöckle et al., 2003), a cropping system model that has been

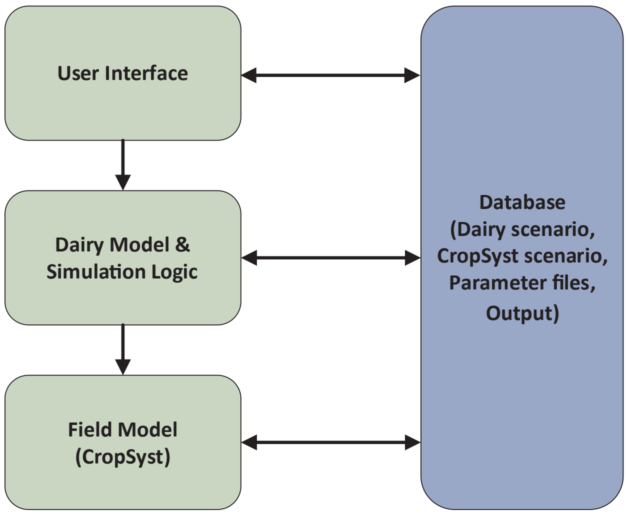

Fig. 3. Relationships among the major components of Dairy-CropSyst. The user interface writes scenario-specific information to the database and executes the dairy models and simulation logic, which in turn executes the field model. Each of the three components can run in isolation if the database is configured properly.

under active development for over 20 years and which has been applied in numerous studies (Donatelli et al., 1997; Pannkuk et al., 1998; Singh et al., 2008; Stöckle et al., 2014). The model has the analytical capabilities to simulate the soil-plant nutrient budget, biomass and crop production, and mineralization of soil organic matter. Lagoon constituents of the manure characterized by the dairy sub model are incorporated into CropSyst biomatter files along with soil, weather, crop rotation, and management files. CropSyst reports biomass, crop yield, nutrient fate and field CO_2 and N_2O emissions.

3. Software architecture

Dairy-Cropsyst consists of three independent executables that communicate through a common database (Fig. 2). The user interface (UI) provides the parameter editor to describe farm facility configurations and operation. The dairy model and associated file input and output logic are contained in a Windows console application coded in C++. The field model, CropSyst, is a Windows console application coded in C++. The database consists of a series of text-based and binary files located on the user's hard drive.

Program flow consists of the following (also see Figs. 3 and 4); parameters describing each of the dairy facilities and equipment operation and scheduling are entered by the user via the user interface (UI). The parameters are stored in a Dairy-CropSyst scenario file. When a crop field is to be simulated, parameters for each field are stored in CropSyst scenario files. Next, the user initiates the run of the model scenario and finally, the user interface displays the results. When the user begins the model run, the UI executes the dairy model and simulation logic. Then the simulation logic reads the scenario and weather data from the database and runs the necessary dairy models and writes emission and nutrient data. If a farm field simulation is specified, the simulation logic writes the fertigation and management information to the database and executes the CropSyst component. Once the dairy models and, optionally, the field model is completed, the simulation logic aggregates output information and creates a summary of the output. Finally, UI informs the user that the simulation has finished and displays the results.

4. Model evaluation

Data on gaseous emissions from dairy farms at various locations in the United States, Canada, and Europe were used for model evaluation. For simulations, essential model input parameters were obtained. These data sets included gaseous emission of NH_3, CH_4, and N_2O from unit operations including barn, lagoon, and manured crop land. Different statistical indices were used to evaluate model performance; their detail and interpretation is provided in Appendix C. A summary of these statistical indices for different emission data sets used in model evaluation is provided in Table 2.

4.1. Barn emission, Sweden

Emissions of NH_3 and CH_4 were measured for 26 days from a dairy barn holding 180 ± 15 dairy cows with an average body weight of 600 kg. The cows were fed twice a day with 20.1 kg dry matter consisting of grass, corn silage, straw, beet pulp, wheat, and protein premix in variable proportions. The barn was naturally ventilated with automatic side curtains for air and temperature control, manure was scraped twice a day from barn during the experimental period. Further details on experimental setup, feed composition, climate data, and barn layout are available in Ngwabie et al. (2009).

Barn CH_4 and NH_3 emission were simulated based on input parameters by specifying herd size, feed intake, barn management, and ambient conditions. Dairy-CropSyst simulated CH_4 emissions from the

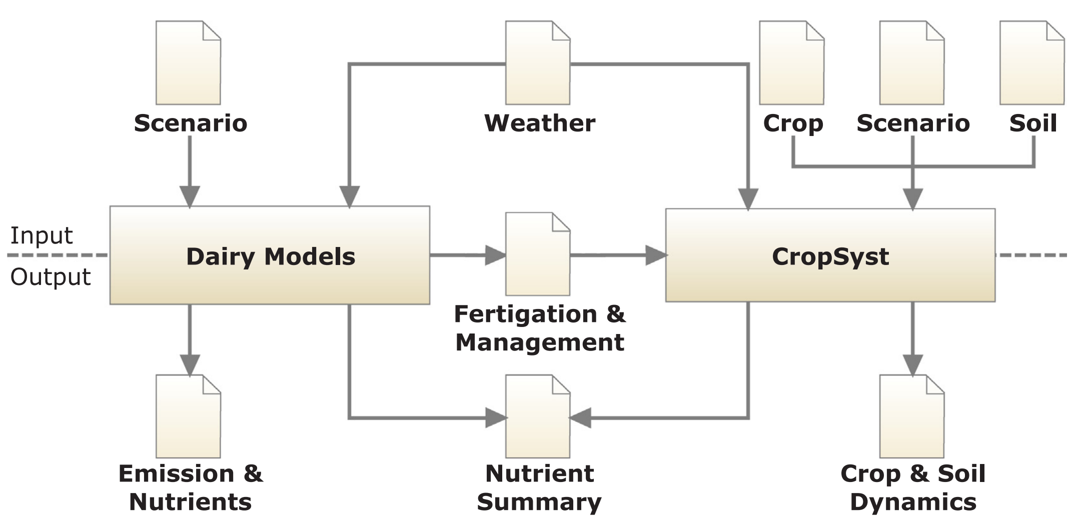

Fig. 4. Data flow among the components of the dairy model and the field model, CropSyst. Files above the dashed line denote input parameter files, those below denote output.

Table 2
Statistical indices of observed and predicted values for different study sites used in model evaluation. Values of NH_3 and CH_4 are in kg d^{-1} cow^{-1} for Sweden and Idaho farms, kg m^{-2} d^{-1} for the Alberta (Canada) farm, and g ha^{-1} d^{-1} for Idaho field N_2O emission.

Study site	Emission	Mean		Statistical Indices[a]					
		Observed	Predicted	RMSE	MAE	CRM	D	NMSE	r
Sweden farm	Barn NH_3	0.0296	0.0289	0.0066	0.0054	0.0233	0.980	0.050	0.64
	Barn CH_4	0.3314	0.3380	0.0218	0.0162	0.0200	0.961	0.004	0.30
Idaho farm[b]	Barn NH_3	0.1520	0.1517	0.0473	0.0393	0.0016	0.996	0.097	0.77
		0.1188	0.0755	0.0555	0.0442	0.3647	0.974	0.344	0.62
		0.0625	0.0451	0.0231	0.0191	0.2777	0.997	0.189	0.79
	Lagoon NH_3	0.2833	0.2356	0.0757	0.1006	0.1686	0.995	0.086	0.56
		0.1988	0.1563	0.0564	0.0462	0.2139	0.989	0.170	0.81
		0.1122	0.0910	0.0318	0.0232	0.1895	0.982	0.085	0.81
	Lagoon CH_4	0.4305	0.4520	0.2899	0.2522	0.0476	0.976	0.431	0.48
		0.8662	0.7871	0.4374	0.3489	0.0546	0.972	0.280	0.73
		0.5431	0.7211	0.2652	0.2001	0.2469	0.995	0.179	0.54
Canada farm	Lagoon NH_3	4.109	3.218	2.0561	1.6784	0.2168	0.996	0.196	0.69
Idaho field N_2O emission[c]	Corn	7.157	12.370	14.609	248.05	−0.728	0.950	2.410	−0.27
	Barley	9.347	11.646	15.969	207.84	−0.246	0.955	2.342	0.17
	Alfalfa	4.333	10.839	11.216	115.99	−1.501	0.962	2.678	0.44

[a] RMSE: Root mean square error, MAE: Mean absolute error, CRM: Coefficient of residual mass, D: Willmott index of agreement, NME: Normalized mean squared error, r: correlation coefficient.
[b] Barn NH_3 emission was measured during July 2009, June 2010, and March 2011, lagoon NH_3 during June, August, and December in 2010, while lagoon CH_4 emissions during August and September 2010.
[c] Statistic doesn't include the emission during the peak irrigation frequencies.

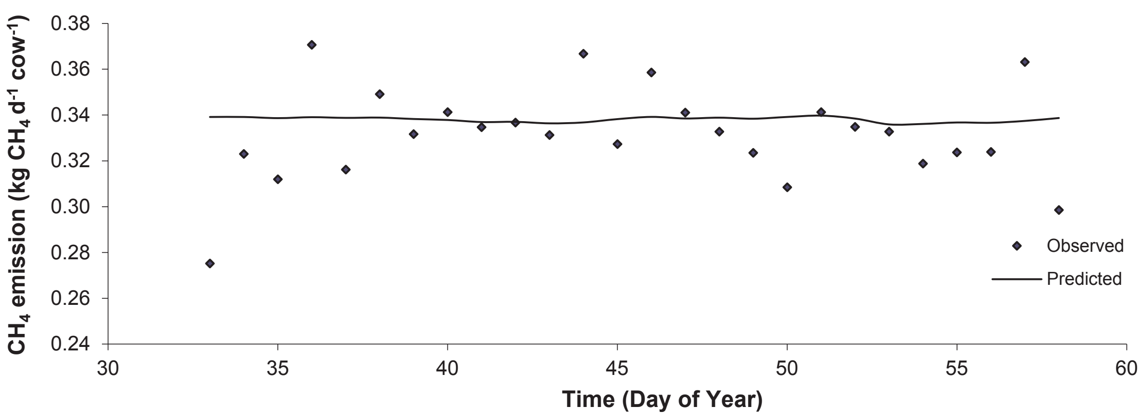

Fig 5. Dairy barn observed and simulated CH_4 emission during 2007 at a dairy facility located in Sweden.

barn were in on average on agreement with observed values (Fig. 5). Modeled CH_4 flux was relatively constant with very little or no diurnal variation compared to the observed values, however, the mean of observed values was fairly close with modeled emission and low normalized mean square error (NMSE) of 0.004 kg CH_4 Cow^{-1} d^{-1}. The model did not capture the variation in CH_4 flux having low correlation (r = 0.30) due to the assumption of constant metabolic processes, but in real time the animal ingesta and metabolic processes varied over time and were responsible for this variation in the observed emissions. A variation of ± 10% in metabolic energy intake encompasses the variation of observed CH_4 fluxes.

Similarly, the simulated NH_3 fluxes from the dairy barn were also in close agreement with the observed fluxes, both in terms of trend and average magnitude (Fig. 6). The small difference of 6×10^{-4} kg NH_3 cow^{-1} d^{-1} between root mean square error (RMSE) and mean absolute error (MAE) indicated a very low variance among the individual errors in the data set. Both the simulated and observed NH_3 flux from the barn floor captured a clear pattern due to variation in the ambient condition mainly driven by temperature and wind speed on the barn floor. Compared to CH_4 a higher correlation (r = 0.64) was found for NH_3 volatilization between observed and model simulated emission.

4.2. Dairy barn and lagoon emission, Idaho, USA

Emissions of NH_3 and CH_4 from a barn and a lagoon on a dairy facility located in southern Idaho were used for model validation. This dairy farm housed 10,000 (± 5%) Holstein cows with an average body weight of about 635 kg. Dairy cows were fed an alfalfa based mixed ration containing 17.6% crude protein and a target dry matter intake of 24 kg cow^{-1} d^{-1}. The herd was kept in six naturally ventilated barns with a total barn area of about 134,640 m^2 (4 barns were 670 m × 40 m and 2 barns were 343 m × 40 m). Barn manure alleys had an area of about 71,359 m^2 and were flushed twice a day. An exercise area was adjacent to each barn, thus total combined area receiving manure was approximately 264,454 m^2. The manure was stored in three lagoons, two measured 200 m × 275 m, while the third smaller lagoon was 150 m × 215 m for a combined total surface area of 142,250 m^2. Before storing manure in the lagoon, it was passed through AD, and coarse fiber was recovered through screen separators. A detailed description of the site, manure management, climate data, and emission measurements protocol is available in Leytem et al. (2013).

Three sets of data for NH_3 emission from the dairy barn measured during the months of March, May, and July during the years 2009–11 were used for model validation. Reasonable agreement was found

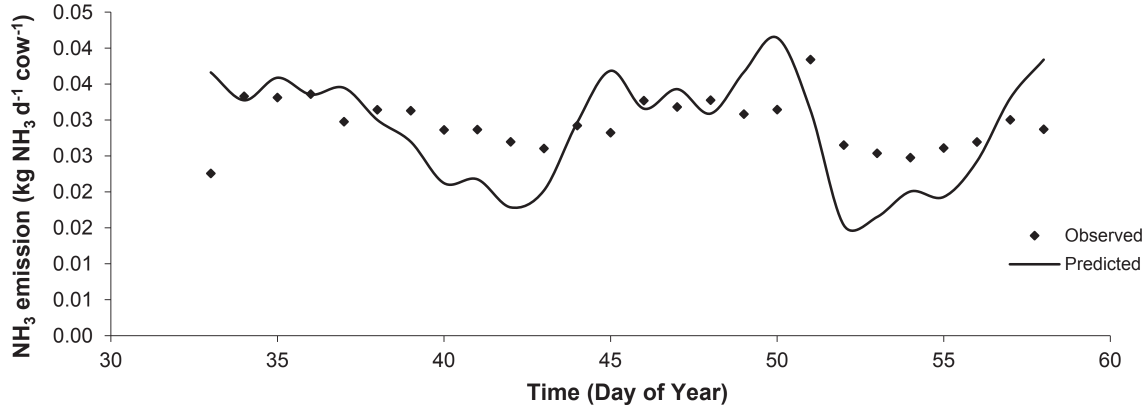

Fig. 6. Dairy barn observed and simulated NH_3 emission during 2007 at a dairy facility located in Sweden.

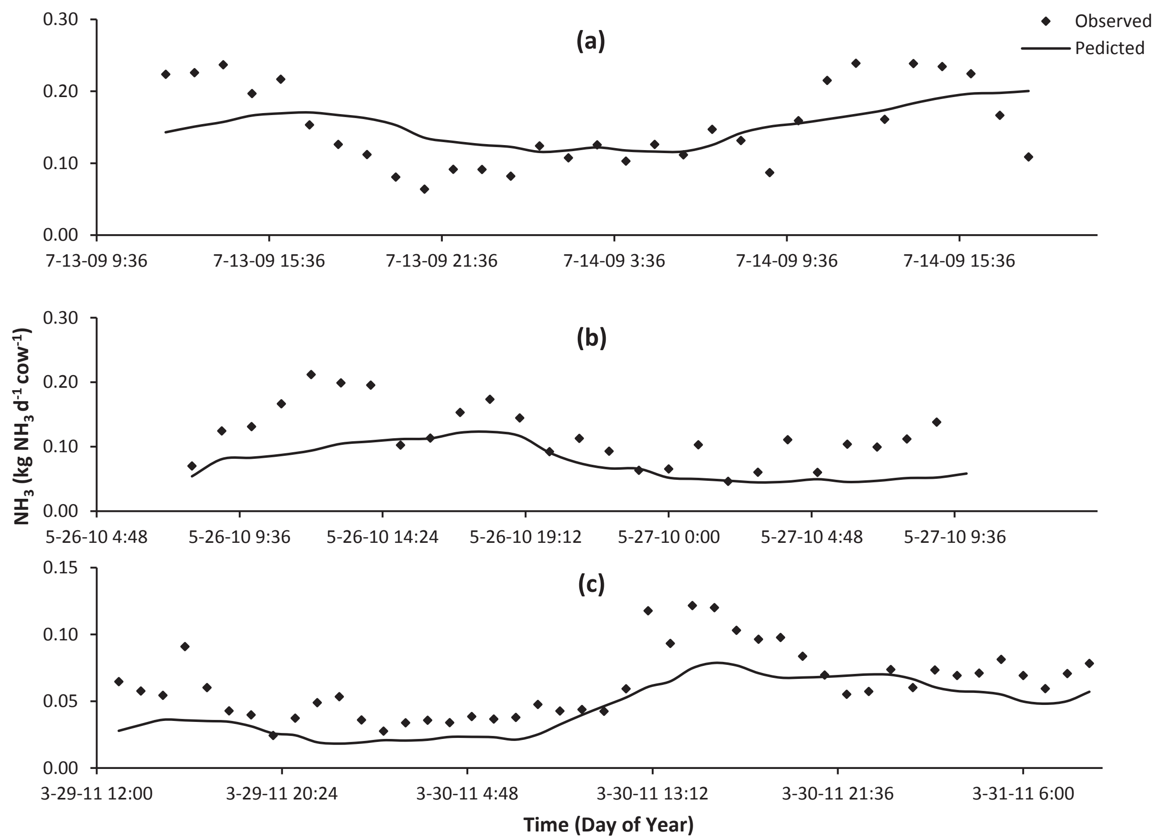

Fig. 7. Observed and simulated NH_3 emission from an open-freestall dairy in Southern Idaho, USA. Hourly averages projected to daily values were measured during: (a) July 2009; (b) August 2010; and (c) March 2011.

between measured and observed NH_3 emission. Simulated average ammonia emission values were very similar in trend and magnitude with observed values. Simulated values showed a clear seasonal variation (Fig. 7), which was mainly attributed to temperature and wind speed.

Emissions had an average NMSE of 0.210 kg NH_3 cow^{-1} d^{-1} for fluxes measured in March, May, and July. The relatively high NMSE when compared to the Sweden dairy barn could be due to the use of hourly averaged values projected to the daily time step. In all three cases the model predictions were lower than observed having an average coefficient of residual mass (CRM) of 0.21, and correspond to the barn missing a flush-event in the observed data when projected to the daily time step. The model predicted NH_3 emission had uniform variance and was in close agreement with observed values.

Simulated and observed lagoon NH_3 emission values during June, August, and September 2010 are presented in Fig. 8. During the observation period, lagoon pH fluctuated between 8 and 8.5, however, corresponding pH values with the observed data points were not recorded. Since NH_3 volatilization is sensitive to pH, the model was first calibrated for pH. For this purpose, about 30% of initial observations from each data set were used for model calibration. Multiple simulations were made changing pH by a factor of 0.25. The pH values corresponding to emissions with least sum of squares between the observed and predicted were used in simulating for the remaining 70% of the data. The model predicted the lagoon NH_3 emission reasonably well, reflecting the effects of diurnal variation in temperature and wind speed. The model had slightly lower values for error and bias, but modeled values were not significantly different from the observed data. The NMSE ranged between 0.085 and 0.170 kg NH_3 cow^{-1} d^{-1} while the CRM ranged between −0.14 to 0.35. A high correlation was found

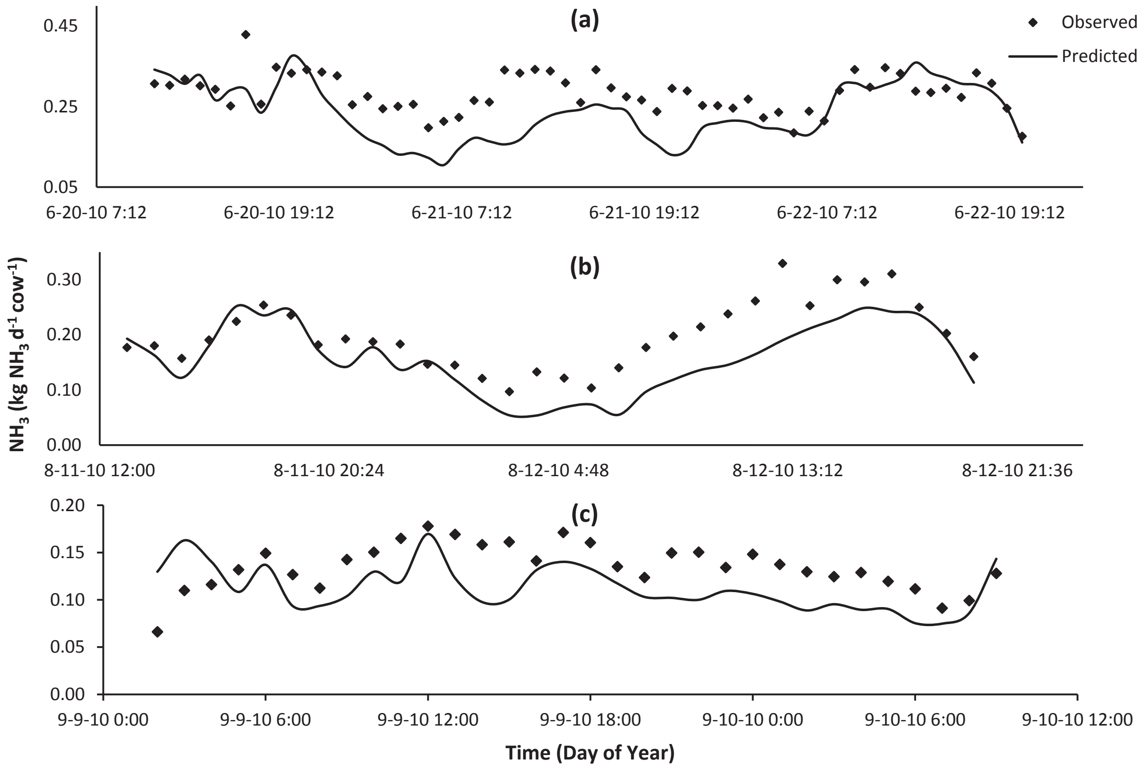

Fig. 8. Southern Idaho lagoon observed and simulated NH_3 emission. Hourly averages projected to daily values were measured during the month of: (a) June; (b) August; and (c) September, during 2010.

between the simulated and observed value.

Simulated and observed CH_4 emission are provided in Fig. 9. Lagoon hourly CH_4 emission validation was carried out in two steps. The model was first run with the average observed temperature data for the period until the lagoon initial conditions were obtained, emitting close to the observed average values. The model was then rerun with calibrated initial conditions reducing the herd size to half to match lagoon manure daily inflow with two barn flush events. The predicted values

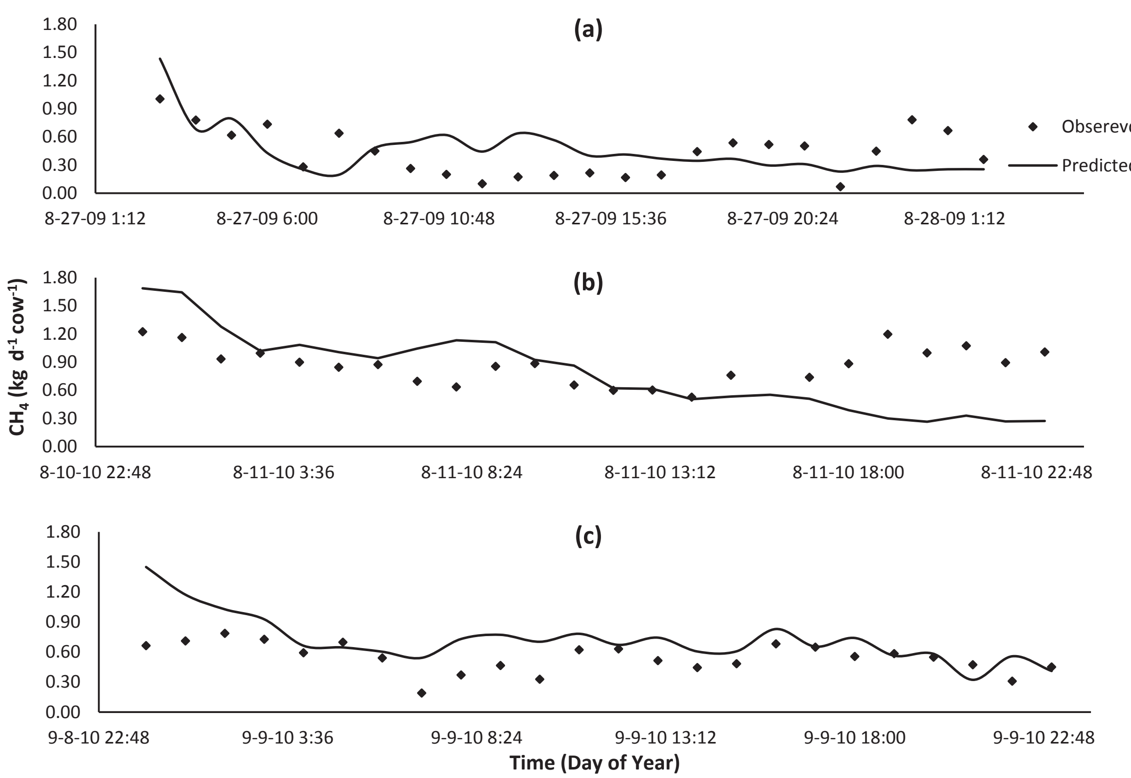

Fig. 9. Sothern Idaho lagoon observed and simulated CH_4 emission. Hourly averages projected to daily values were measured during the month of: (a) August 2009; (b) August 2010, and (c) September 2010.

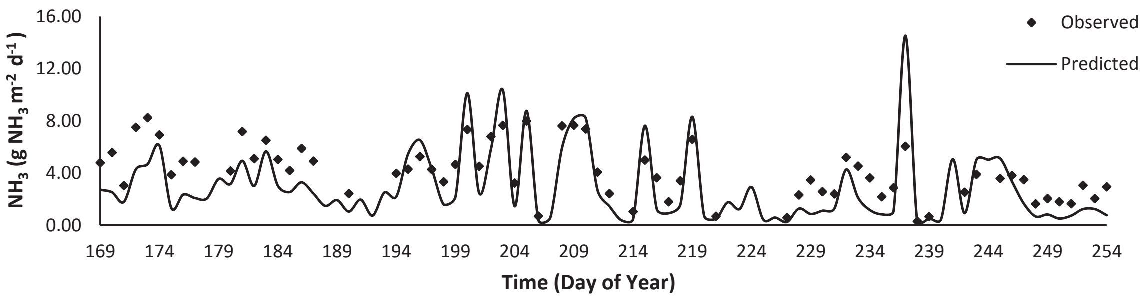

Fig. 10. Observed and predicted lagoon NH_3 emissions during summer 2007 at a dairy facility located in Alberta, Canada.

had good agreement with the observed readings (Fig. 9) with average index of agreement (D) value of 0.98. The predicted values had an overall consistent agreement with the observed values. The model responded well to temperature effect on C mineralization.

4.3. Dairy lagoon emissions, Canada

The dairy farm on which these data were obtained had 150 lactating Holstein cows in a naturally ventilated barn. Manure was scraped from barn alley, stored in a temporary storage tank located underneath the barn floor, and periodically pumped out from the barn storage tank to the lagoon located 290 m from the barn. The total storage capacity of the lagoon was 10800 m^3 with a surface area of 3198 m^2 and berm height of 2 m from ground surface. The lagoon was surrounded by a flat surface and there was no obstruction to wind flow. Further details on biochemical composition, farm management, and ammonia volatilization procedures are available in McGinn et al. (2008).

The observed and predicted NH_3 emissions data are presented in Fig. 10. The model simulation both in terms of magnitude and pattern were in close agreement with the observed data. The observed and predicted data had fairly uniform residual errors and low level of bias, showing good model performance. The model net NH_3 were lower than the observed and may be attributed due to upstream TAN concentration from the auxiliary storage pond between the barn and main lagoon. The simulated NH_3 emission captured the diurnal variation mainly driven by ambient conditions when compared to observed values.

4.4. Emissions from a manured field, Idaho, USA

Nitrous oxide emissions data from a manured field at the USDA-ARS Northwest Irrigation and Soils Research Laboratory, Kimberly, Idaho was used to validate the field component of the model. The soil at the field site was classified as silt loam (Portneuf series) which was subject to conventional tillage practices and partial crop residue removal. Solid dairy manure collected from a local dairy was applied in fall 2012 and 2013 to the experimental field at an average rate of 1067 and 1197 kg N ha^{-1} respectively. The crops during the experimental period were corn, barley, and alfalfa. Irrigation water was applied using a lateral-move system and received net irrigation of 600, 420, and 615 mm in 2013, 2014, 2015 respectively. The N_2O gas samples were collected using vented, non-steady-state, closed chambers following the USDA-ARS GRACEnet protocols (Parkin and Venterea, 2010). Chamber sampling was conducted periodically during the crop growing season at 10:00 ± 1 h for a 30-min period and projected to daily time step. Complete details from this study are available in Dungan et al. (2017)

Model evaluation was performed with the assumption that manure was uniformly spread on the field and measured chamber emissions were representative of the whole plot. Fig. 11 shows Dairy-CropSyst simulated and observed daily N_2O fluxes for three consecutive cropping periods of 2013–15. The simulated N_2O fluxes and corresponding observed values were in close agreement before and after the period of frequent irrigation. During the intense irrigation period, chamber sampling would have to have been much more frequent and more closely associated with irrigation events to expect a tight correlation between simulated and measured N_2O emissions. However, the chamber sampling was not conducted intensively throughout the day during and after the irrigation events, as this study had been designed for a different purpose but not directly for validation of this model. Our model predicted a response to N_2O emission during the peak irrigation period that was similar to Trost et al. (2013) who reported that the N_2O emissions were positively correlated to irrigation and precipitation events. Also in irrigated fields studied in Asia, N_2O flux from the soil was at a minimum just prior to irrigation, and then spiked very quickly after irrigation (Scheer et al., 2008). In another study, Dairy-CropSyst N_2O emission spikes after irrigation events were also found to be similar to those reported by Cai et al. (2003) where N_2O fluxes from onion fields were driven predominately by rainfall.

5. Sensitivity analysis

5.1. Impact of manure management practices and biochemical properties of manure

An analysis was made to determine the impact of selected alternative management options and biochemical properties of manure on NH_3 and GHG emissions. These options and properties included different animal feed composition, physical farm configurations, manure management options, and changes in manure biochemical properties. Parameters for the various treatments were obtained from the literature and technical user manuals developed for dairy operations. A hypothetical scenario was created to mimic a representative dairy located in the Yakima Valley of central Washington where most of the state's large dairies are located. The output of the test scenarios was influenced by the herd size, feed type and intake, and farm management practices. The model input parameters common to all scenarios are provided in Table 3. In test scenarios, simulation maximum and minimum values available in the literature were used for the input parameter whose impact was in question, while the rest of the input parameters were kept constant using their typical values. The impact of selected input parameters was assessed as percent change in GHG and NH_3 emission from barn and lagoon components. Response of gaseous emissions to different factors from barn and lagoon unit operation is summarized in Table 4.

The results showed that an increase in feed crude protein content had a significant impact on NH_3 volatilization, particularly from the barn and subsequently from the lagoon, but had no significant impact on GHG emission. The increase in volatilization was mainly attributed to an increase in urine N, which usually hydrolyzes rapidly to ammonium compared to organic N found in the fecal matter. The crude protein increase in food also increased the lagoon emission, but the proportion was lower than the barn (Table 4). The lagoon NH_3 emission, however, could be further triggered if the lagoon ambient condition is windy. The available diet acid detergent fiber fraction (ADF) had no significant impact on GHG emission and was predominantly

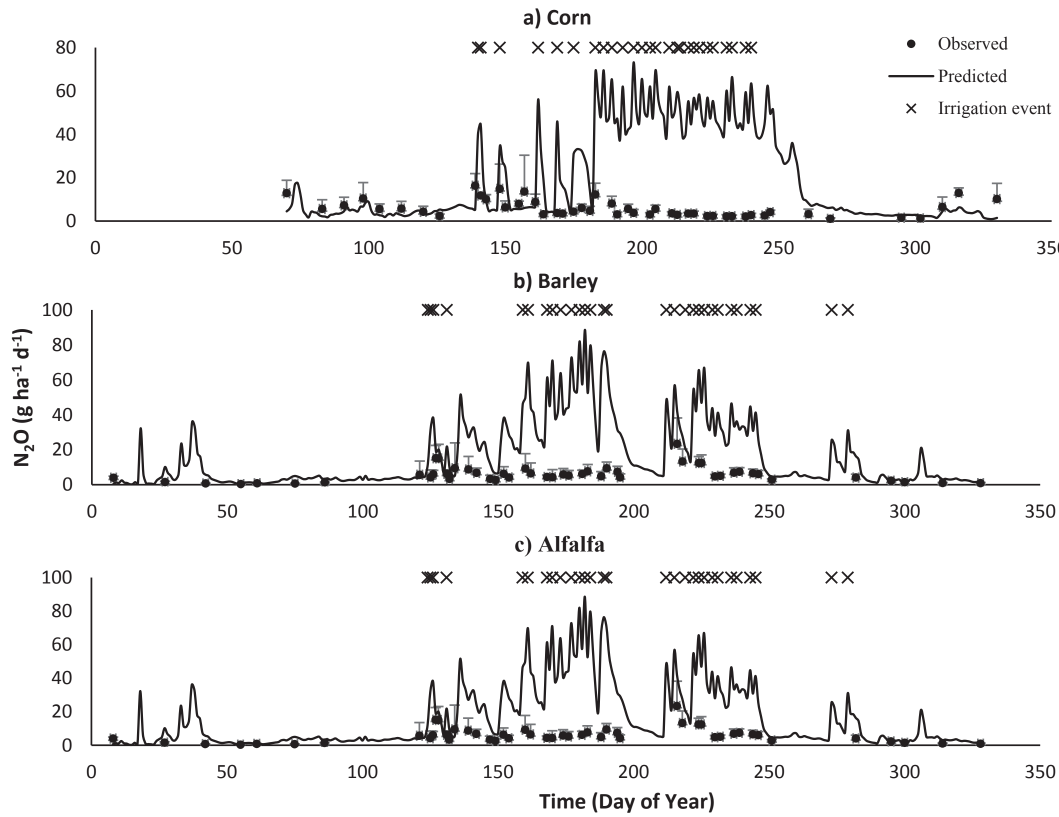

Fig. 11. Observed and simulated N_2O emissions from dairy manure application during fall 2012–13 for corn-barely-alfalfa crop rotation. The error bar on the observed values represent standard deviations from means.

Table 3
Test scenario model input parameters for a study of the impact of farm management alternatives on modeled emissions from dairy CAFOs. The values selected are based on values found in literature or common to the dairy facilities in the Pacific Northwest of the United States.

Description	Value
Herd size	1000 cows
Body weight	635 kg
Dry matter intake	24 kg d^{-1} cow^{-1}
Diet crude protein	16.7%
Milk production	34 kg d^{-1} cow^{-1}
Metabolic energy in diet	150 MJ cow^{-1} d^{-1}
Diet starch fraction	15%
Diet acid detergent fiber fraction	26%
Barn cleaning frequency	3 d^{-1}
Barn manure alley area	2.25 m^2 cow^{-1}
Maximum manure holding capacity of lagoon	50 m^3 cow^{-1}
Lagoon depth	4 m
Manure fertigation	91 day of year
Manure volume pumped out during fertigation	90%
Fertigation frequency	90 day

attributed to the low variability (i.e. 4%) of ADF values recommended in dairy feed.

The barn physical configuration and operational parameters also affected the barn NH_3 emission. Increasing the barn alley from 1.85 to 2.60 m^2 cow^{-1} increased NH_3 barn emissions, but had little effect on subsequent lagoon NH_3 emissions (Table 4). Barn alley cleaning frequency affected NH_3 emission, with an increase in cleaning frequency from 2 to 4 scrapes per day reducing NH_3 volatilization by more than 20%. Barn cleaning frequency had no significant impact on lagoon emissions. Among the manure treatments the effect of AD on gaseous emission was analyzed. Though AD manure treatment reduces the risk of carboneous emission, it increases the TAN and pH of the effluent which increases NH_3 volatilization during lagoon storage. A comparison of test scenarios shows that NH_3 volatilization from lagoon storage increased by more 1.8 times with AD treatment. This increase suggests that NH_3 recovery techniques should be implemented in conjunction with AD both to minimize air quality concerns and to maximize nitrogen recovery.

The lagoon emptying frequency was negatively correlated with both NH_3 and GHG emissions due to reduced storage time with less chance to release gaseous emission. More frequent fertigation (i.e. lagoon emptied 4 times a year) reduced NH_3 and net GHG emissions by 26 and 15%, respectively, when compared to two fertigation events per year (Table 4). The N losses during field application were estimated using an emission factor for different method of manure field application, scenarios evaluation shows that N losses were not much affected when the fertigation frequency was changed from 2 to 4 per year. The lagoon and barn dimensions also affected NH_3 volatilization; an inverse relationship was found when the depth of lagoon was changed from 3 to 6 m. The decrease in NH_3 volatilization with increase in lagoon depth was expected as the NH_3 emission are positively correlated with surface area following convective mass transfer law. There was no effect on total C mineralization by changing the lagoon configuration, because the decomposition process is modeled as first order kinetics where the emissions are independent of the surface area.

5.2. *Impact of mass transfer coefficients*

A sensitivity analysis of mass transfer coefficients was also performed to estimate the variations in model outputs. The model was run numerous times changing one parameter at a time and analyzing the outputs using the approach out line in Jørgensen and Fath (2011). Parameters that showed more variability in the model outputs in the preliminary runs, were included in the analysis. Parameters included in the analysis were: maximal rate of urea nitrogen conversion (r_{max_urea}),

Table 4
Impact of farm alternative management practices on GHG and NH_3 emission from barn and lagoon. Upper and lower limits were either based on values available in literature or using farms typical in the United States.

Unit Operation	Factor	Level	Response	(Percent Change)	
				Barn	Lagoon
Feed	Crude Protein	14% 21%	NH_3_N (kg)	80	20
	ADF	26% 30%	GHG (CO_2_eq)	2	–
Barn	Alley Area	$1.85\ m^2\ cow^{-1}$ $2.60\ m^2\ cow^{-1}$	NH_3_N (kg)	38	−2
	Cleaning Frequency	2 per day 4 per day	NH_3_N (kg)	−21	1
Manure treatment	Biochemical composition [a]	(No AD) (AD)	NH_3_N (kg)	–	183
Lagoon	Fertigation frequency	2 per year 4 per year	GHG (CO_2_eq)	–	−15
		2 per year 4 per year	NH_3_N (kg)	–	−26
	Lagoon Depth	3 m 6 m	NH_3_N (kg)	–	−33

[a] Assuming an increases in pH by 0.5 and TAN by 25% when manure is getting treated by AD.

half time saturation constant for oxygen (K_{DO}), maximal rate of nitrification (r_{Nit_max}), adapted acid dissociation constant for NH_3 (K_a), half time saturation constant for urea conversion (K_{urea}), and decomposition rate for the residue and microbial pool (k_{dec}). The sensitivity of an input parameter (S) on a model output was tested as the ratio between the change in the output to the change in the input parameter. The model was run numerous times changing one parameter at a time and analyzing the outputs.

K_{DO} shows sensitivity on N_2 and N_2O emissions when K_{DO} is reduced 50%. Low values of K_{DO} reflect a higher ability of the nitrifying bacteria to compete for the available oxygen with other microorganisms, increasing nitrification rates. Conditions in the lagoon favor denitrification, which is mostly limited by the availability of NO_3 in the lagoon. The most sensitive parameter in NH_3 volatilization was found to be K_a. A higher concentration of NH_3 in aqueous solution (higher K_a) directly increases NH_3 volatilization. In terms of C losses (both CO_2 and CH_4) in the lagoon, the most sensitive parameter is k_{dec}, which has a direct influence in how fast the organic residues present in manure are decomposed to form CO_2 and CH_4. Careful selection of K_{DO}, r_{Nitr_max} and K_a and k_{dec} residue values is required before running the model.

6. Concluding remarks

Dairy-CropSyst could assist the global dairy industry in making nutrient management decisions. The model is useful in matching crop nutrient requirements with manure application on the available crop land and has the capability to estimate the amount of surplus nutrients recovered through manure treatment options that could be stored, reused, and/or transported to other farms. Dairy-CropSyst demonstrates the effect of manure treatment options with respect to gaseous emissions starting from the animals to land application of the manure. This information could be used in EPA's GHG reporting program and to assess suitable animal-to-land ratios without exceeding the soil nutrient carrying capacities under the farm-specific Comprehensive Nutrient Management Plan. Since the model's subroutine uses accepted equations, kinetics, and dairy practices that could be also used worldwide on dairies with liquid manure handling system with slight adjustments. Further modification/adoption could allow the model application to other livestock operations. Overall, the Dairy-CropSyst model has the potential to streamline a farmer's management of dairy manure thus benefitting crops, soil, and the environment. The model, and its user manual is available for download at: http://modeling.bsyse.wsu.edu/CS_Suite_4/.

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Appendix A

Model processes characterizing dairy manure nutrients and emissions.

Description	Equation	Reference
Manure Production	$M_{exc} = 0.647 \times MP + 43.212$	(ASABE, 2005)
Manure Excreted	M_{exc} = manure excreted by dairy cow (kg d^{-1} cow^{-1})	(Nennich et al., 2005)
	MP = Milk production (kg d^{-1} cow^{-1})	
Urine Excreted	$U_{exc} = 0.017 \times BW + 11.704$	
	U_{exc} = Urine excreted (kg d^{-1} cow^{-1})	
	BW = Dairy cow body weight (kg)	
Dry Matter Excreted	$DM_{exc} = 0.35 \times DM_I + 1.017$	
	DM_{exc} = Dry matter in manure (kg d^{-1} cow^{-1})	
	DM_I = Dry matter intake (kg d^{-1} cow^{-1})	
Manure Nutrients	$N_{exc} = (4.204 \times MP + 283.3)/1000$	(Bannink et al., 1999)
Nitrogen Excreted	N_{exc} = Total nitrogen excreted in manure (kg d^{-1} cow^{-1})	(de Boer et al., 2002)
Urine Nitrogen	$N_{urine} = [75.18 + 0.719(-42.5 + 734 \times N_{diet} + 1000 \times N_{milk})]/1000$	(NRC, 2001)
	N_{urine} = Nitrogen in urine (kg)	(ASABE, 2005)
	N_{diet} = Nitrogen in animal diet (kg)	(Nennich et al., 2005)
	$N_{diet} = 0.16(\frac{CP_{diet}}{100} \times DM_I)$	
	CP_{diet} = Crud protein in animal diet (%)	
	N_{milk} = Nitrogen in milk (kg)	
	(Fresh milk contains about 3.2% of crude protein and 15.7% of it is considered to be nitrogen)	
Carbon Excreted	$C_{exc} = N_{exc} \times C{:}\ N$	
	C_{exc} = Carbon excreted in manure (kg d^{-1} cow^{-1})	
	C:N = Carbon nitrogen ratio in fresh manure	
Phosphorus Excreted	$P_{exc} = (0.773 \times MP + 46.015)/1000$	
	P_{exc} = Phosphorous excreted in manure (kg d^{-1} cow^{-1})	
Potassium Excreted	$K_{exc} = (1.8 \times MP + 31.154)/1000$	
	K_{exc} = Potassium excreted in manure (kg d^{-1} cow^{-1})	
Dairy Barn EmissionCarbon Dioxide	$CO_{2Barn} = N \times CO_{2resp} + A \times CO_{2floor}$	(Kirchgessner et al., 1991)
	$CO_{2resp} = -1.4 + 0.42 \times DM_I + 0.0045 \times BW^{0.75}$	(Rotz and Chianese, 2008)
	$CO_{2floor} = \max(0, 0.05075 + 0.00185 \times T_{air})$	
	$CO_{2\ resp}$ = Carbon dioxide respired by dairy cow (kg d^{-1} cow^{-1})	
	$CO_{2\ floor}$ = Carbon dioxide emitted from manure on barn floor (kg d^{-1} m^{-2})	
	N = Number of dairy cows	
	A = Area of barn manure alley (m^2)	
	T = Temperature (°C)	
Methane	$CH_{4Barn} = N \times CH_{4resp} + A \times CH_{4floor}$	
	$CH_{4resp} = 0.018 \times (E_{max} - E_{max} \times e^{-cME})$	
	$c = -0.0011 \times \frac{Starch_f}{ADF_f} + 0.0045$	
	$CH_{4floor} = \max(0, 0.029 + 0.14 \times T_{air})$	
	E_{max} = 45.98 (MJ CH_4 $head^{-1}$ d^{-1})	
	ME = Metabolized energy intake (MJ $head^{-1}$ d^{-1})	
	$CH_{4\ resp}$ = Dairy cow enteric fermentation methane emission (kg d^{-1} cow^{-1})	
	$CH_{4\ floor}$ = Methane emitted from manure on barn floor (kg d^{-1} m^{-2})	
	$Starch_f$ = animal feed starch fraction	
	ADF_f = Acid detergent fiber fraction in feed	
Urea Hydrolysis	$r_{urea} = \frac{r_{max\_urea} \times \lvert Urea \rvert}{K_{urea} + \lvert Urea \rvert} \times V$	(Monteny et al., 1998)
	r_{urea} = Urea hydrolysis (kg d^{-1})	
	r_{max_urea} = 0.162 (kg m^{-3} min^{-1})	
	$\lvert Urea \rvert$ = Urea N concentration (kg N m^{-3})	
	K_{urea} = 0.056 (kg N m^{-3})	
	V = volume of manure (m^3)	
NH_3 Volatilization	$\Phi_{barn} = \frac{[k \times A_{barn} \times f \times TAN]}{H}$	
	Φ = ammonia volatilization (kg N d^{-1})	
	A = lagoon surface area	
	k = ammonia mass transfer coefficient (m d^{-1})	
	f = fraction of ammonia nitrogen in TAN	
	TAN = Total ammonium N concentration (kg N m^{-3})	
	H = Henry constant	
	$k = 0.1842 \times ws^{0.8} \times (T_{barn} + 273)^{-0.4} \times 1440$	
	$f = \frac{1}{1 + \frac{10^{-pH}}{K_a \times 1.07^{(T-20)}}}$	
	$H = 1384 \times 1.053^{(20-T)}$	
	T_{barn} = barn ambient temperature (°K)	
	pH = manure pH	
	K_a = adapted acid dissociation constant for NH_3 (dimensionless)	
	T = manure temperature (°C)	
	ws = wind speed at the barn floor (m s^{-1})	

Lagoon Processes and EmissionCarbonMineralization	$C_{min} = f_T \times f_{DO}(k_l \times C_l + k_s \times C_s + k_r \times C_r)$ C_{min} = Carbon Mineralized (kg d^{-1}) f_t = temperature correction factor f_{DO} = dissolved oxygen correction factor k = decomposition rate constant (d^{-1}) C = Carbon (kg) Subscript "l" = labile pool Subscript "s" = slow pool Subscript "r" = recalcitrant pool Where $f_t = \max[0, (2.32^2 \times T^2 - T^4/32^4)]$and $f_{DO} = \max[0, \frac{maxDOana - DO}{maxDOana + DO}] + \max[0, \frac{DO - minDOan}{DO + minDOna}]$ DO = Dissolved oxygen (mg l^{-1}) $maxDO_{ana}$ = Maximum dissolved oxygen at which anaerobic decomposition stops (i.e. 1 mg l^{-1}) $minDO_{ana}$ = Mimimum dissolved oxygen at which aerobic decomposition stops (i.e. 0.1 mg l^{-1})	(Paul et al., 1999) (Schomberg et al., 2002) (Asaeda et al., 2000)
Nitrification	$r_{Nitr} = r_{maxNitr} \times C_T \times C_{pH} \times \left(\frac{\lvert NH4\rvert}{\lvert NH4\rvert + K_{NH4}}\right) \times \left(\frac{DO}{K_{DO} + DO}\right) \times V$ r_{Nitr} = nitrification rate (kg N m^{-3}) $\lvert NH4\rvert$ = ammonium concentration (kg N m^{-3}) K_{NH4} = half time ammonium saturation constant (1 kg N m^{-3}) K_{DO} = half time DO saturation constant (2 mg l^{-1}) C_T = Temperature correction factor $C_T = e^{0.098(T-15)}$ C_{pH} = pH correction factor $C_{pH} = \begin{matrix} 1 - 0.833(7.2 - pH) \text{If} 6.0 \le pH < 7.2 \\ 1 \text{If} pH \ge 7.2 \end{matrix}$	Kadlec and Knight (1996)
Denitrification	$r_{Denit} = k_{Denit-20C} \times$ Ó̈ $\times \lvert NO_3\rvert \times V$ r_{Denit} = denitrification rate (kg N d^{-1}) $\lvert NO_3\rvert$ = nitrate concentration (kg N m^{-3}) V = volume of manure(m^3) Θ = temperature function $\theta = 1.09^{(T-20)}$	Kadlec and Knight (1996)
N_2O EmissionNH_3 Emission	$N_2O = r_{N2O_{Dnitr}} + r_{N2O\_Nitr}$ $r_{N2O\_Nitr} = \lvert NO_3\rvert_i \times (-0.0005 \times T + 0.0126)$ $r_{N2O\_Dnitr} = \frac{r_{Denitr}}{1 + R_{\frac{N2}{N2O}}}$ r_{N2O_Nitr} = N_2O emitted during Nitrification (kg N d^{-1}) r_{N2O_Dnitr} = N_2O emitted during denitrification (kg N d^{-1}) k_{Denit_20C} = denitrification rate at 20 °C (0.57 d^{-1}) r_{Deni} = total denitrification (kg N d^{-1}) $R_{N2/N2O}$ = ratio of di-nitrogen to nitrous oxide $R_{\frac{N2}{N2O}} = 23.5 \times [\frac{1.4}{13\ (\frac{17}{13^{2.2}})}]$ $\Phi_{lagoon} = \frac{[k \times A_{lagoon} \times f \times TAN]}{H}$ Φ = ammonia volatilization (kgN d^{-1}) A = lagoon surface area k = ammonia mass transfer coefficient (m d^{-1}) f = fraction of ammonia nitrogen in TAN TAN = Total ammonium N concentration (kgN m^{-3}) H = Henry constant $k = 0.1842 \times ws^{0.8} \times (T_{air} + 273)^{-0.4} \times 1440$ $f = \frac{1}{1 + \frac{10^{-pH}}{K_a \times 1.07^{(T-20)}}}$ $H = 1384 \times 1.053^{(20-T)}$ ws = wind speed over the lagoon surface (m s^{-1}) T_{air} = air temperature (°K) pH = manure pH K_a = adapted acid dissociation constant for NH_3 (dimensionless) T = manure temperature (°C). $ws = w(h) \times \ln[\frac{z - h}{zm}]$ z = height over the lagoon exchange surface (m) w(h) = wind speed measured by weather station installed at height h (m s^{-1}) h = weather instrument height (m) z_m = momentum roughness parameter (m)	(Maag and Vinther, 1996) (Parton et al., 1996)

Volume Balance	$V_{(lagoon)i} = V_{(lagoon)i-1} + V_{(in)i} - V_{(out)i} - V_{loss} + PPT$ $V_{(lagoon)i}$ = volumeoflagoononcurrentday $V_{(lagoon)i-1}$ = volumeoflagoononpreviousday $V_{(in)i}$ = Volumerecievedbylagoon $V_{(out)i}$ = volumepumpedoutoncurrentday V_{loss} = EvaporationandSeepagelosses $V_{loss} = \left[\frac{0.622U_rCe}{R_dTs}(e_s - e_a)\right] + \left[\frac{K_S}{A}\left\{A_s\left(\frac{H}{2L}+1\right) + A_b\left(\frac{H}{L}+1\right)\right\}\right]$ PPT = Precipitation es = saturation vapor pressure at the temperature of the water surface (Pa) ea = vapor pressure of the air (Pa) Rd = gas constant ($287.04\ J\ kg^{-1}\ K^{-1}$) Ts = temperature of the surface (K) Ur = wind speed at 1 m ($m\ s^{-1}$) 0.622 = ratio of the molecular weights of water and dry air Ce = bulk transfer coefficient (dimensionless, 2.8×10^{-3}) A = area of the liquid surface (m^2) Ks = saturated hydraulic conductivity ($m\ s^{-1}$) H = waste depth above the bottom of the lagoon (m) As = areal area of the submerged side embankments (m^2). Ab = areal area of the flat bottom (m^2).	(Ham, 2002)

Appendix B

Mass balance of manure flow subject to different treatments. Tabled data were compiled by coauthors (Frear and Ma, 2015) under Cooperative Agreement No. RD-83556701 with the United States Environmental Protection Agency (EPA) as a separate part of the current study.

Wet Cow Equivalent Per Year	Unit	Feces & Urine	Parlor Water	Into Digester	Out of Digester	Out of Screens	Out of DAF[1]	Out of NH_3 Stripper
Manure Wet	MT cow^{-1} $year^{-1}$	23.874	23.924	47.798	46.758	42.425	39.463	33.570
Water Mass	MT cow^{-1} $year^{-1}$	20.770	23.766	44.536	44.536	41.092	38.913	33.076
Total Solids (TS)	MT cow^{-1} $year^{-1}$	3.104	0.219	3.323	2.222	1.333	0.550	0.494
Volatile Solids (VS)	MT cow^{-1} $year^{-1}$	2.606	0.146	2.752	1.651	0.832	0.424	0.368
Fixed Solids (FS, Ash)	MT cow^{-1} $year^{-1}$	0.498	0.073	0.570	0.570	0.501	0.126	0.126
Total Nitrogen (TN)	MT cow^{-1} $year^{-1}$	0.090	0.014	0.104	0.104	0.092	0.062	0.027
Total Kjieldahl Nitrogen (TKN)	MT cow^{-1} $year^{-1}$	0.090	0.014	0.104	0.104	0.092	0.062	0.027
Total Organic Nitrogen (TON)	MT cow^{-1} $year^{-1}$	0.046	0.009	0.055	0.041	0.037	0.012	0.012
Total Ammonia Nitrogen (TAN)	MT cow^{-1} $year^{-1}$	0.044	0.005	0.049	0.063	0.055	0.050	0.015
Total Nitrate/Nitrite Nitrogen	MT cow^{-1} $year^{-1}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total Phosphorus (TP)	MT cow^{-1} $year^{-1}$	0.027	0.003	0.030	0.030	0.027	0.005	0.005
Water-Extractable-Phosphorus (WEP)	MT cow^{-1} $year^{-1}$	0.015	0.001	0.017	0.010	0.004	0.005	0.005
Total Carbon (TC)	MT cow^{-1} $year^{-1}$	1.408	0.094	1.502	0.901	0.541	0.326	0.309
Total Organic Carbon (TOC)	MT cow^{-1} $year^{-1}$	1.382	0.092	1.474	0.883	0.523	0.308	0.308
Total Inorganic Carbon (TIC)	MT cow^{-1} $year^{-1}$	0.026	0.002	0.028	0.018	0.018	0.018	0.001
Total Potassium (TK)	MT cow^{-1} $year^{-1}$	0.056	0.000	0.056	0.056	0.050	0.048	0.048
C/N Ratio		15.645	6.519	14.390	8.634	5.893	5.283	11.588
Organic C/N Ratio		15.354	6.398	14.122	8.461	5.697	4.991	11.547
% Solids	%	13.000	0.915	6.951	4.752	3.142	1.393	1.471

[1]DAF = Dissolved Air Flotation.

Appendix C

Statistical indices used in model evaluation

Statistical Index	Formula	Range	Optimal Value
Mean absolute error (MAE)	$MAE = \sum_{i=1}^{n}(P_i - O_i)/n$	≥ 0	0
Root mean square error (RMSE)	$RMSE = \sqrt{\sum_{i=1}^{n}(P_i - O_i)^2/n}$	≥ 0	0
Coefficient of residual mass[a] (CRM)	$CRM = 1 - \frac{\sum_{i=1}^{n}P_i}{\sum_{i=1}^{n}O_i}$	≤ 1	0
Willmott index of agreement (D)	$D = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(\lvert P_i - \bar{O}\rvert + \lvert O_i - \bar{O}\rvert)^2}$	0 − 1	1
Normalized mean square error (NMSE)	$NMSE = \frac{1}{N}\frac{\sum_{i=1}^{n}\lvert P_i - O_i\rvert}{\bar{O}\ \bar{P}} \times 100$	$\geqslant 0$	0
Pearson correlation coefficient (r)	$r = \frac{\sum_{i=1}^{n}(O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2}\sqrt{\sum_{i=1}^{n}(P_i - \bar{P})^2}}$	−1	1

P_i, predicted; O_i, observed; $\bar{O}$, average observed; $\bar{P}$ average predicted; n, number of observations.

[a]If CRM < 0 the model overestimates. If CRM > 0 the model underestimates.

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