

Manure-DNDC: a biogeochemical process model for quantifying greenhouse gas and ammonia emissions from livestock manure systems

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Abstract From the point of view of biogeochemistry, manure is a complex of organic matter containing minor minerals. When manure is excreted by animals, it undergoes a series of reactions such as decomposition, hydrolysis, ammonia volatilization, nitrification, denitrification, fermentation etc., from which carbon dioxide (CO₂), nitrous oxide (N₂O), methane (CH₄) and ammonia (NH₃) can be produced. Based on the principles of thermodynamics and reaction kinetics, these reactions are commonly controlled by a group of environmental factors such as temperature, moisture, redox potential, pH, substrate concentration gradient etc. The relations among the environmental factors, the reactions and the gas production have been incorporated in a process-based model, Manure-DNDC, to describe manure organic matter turnover and gas emissions. Using Manure-DNDC, the users can construct a virtual farm by selecting and

integrating one or more of the candidate farm facilities (i.e., feedlot, compost, lagoon, anaerobic digester and cropping field) parameterized in the model. Manure-DNDC calculates variations of the environmental factors for each component facility based on its technical specifications, and then utilizes the environmental factors to drive the biogeochemical reactions. To verify the applicability of Manure-DNDC for livestock farms, seven datasets of air emissions measured from farms across the U.S. plus a Scotland pasture were utilized for model tests with encouraging results. A dairy farm in New York was used to assess the impacts of alternative management practices on the gas mitigation. The modeled results showed that a combination of changes in the feed quality, the lagoon coverage and the planted crop type could reduce greenhouse gas emission by 30 % and NH₃ by 36 % at the farm scale.

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Introduction

Agriculture contributes about 20 % of the total anthropogenic greenhouse gas (GHG) emissions (IPCC 1996a). Animal feeding operations are an important source of pollutants affecting local air quality by ammonia (NH₃) volatilization as well as the global atmosphere through methane (CH₄), nitrous oxide (N₂O), nitric oxide (NO) and carbon dioxide (CO₂) emissions. For example, intensive livestock operations account for approximately 50 % of the agricultural CH₄ emissions (IPCC 1996b). The total N₂O emission from the world livestock systems is estimated as high as 1.5–2.7 Tg N, which contribute as much as 30–50 % to the global N₂O emissions from agriculture (Mosier et al. 1998a, b; Oenema et al. 2005). Bouwman et al. (1997) estimated 22–32 Tg NH₃-N was emitted from animal agriculture to the atmosphere in 1990. Over 34.4Tg of manure N are excreted globally every year (Sheldrick et al. 2003); and projections by FAO suggest that livestock numbers will increase by 40 % between 2000 and 2030. As the environmental impacts of livestock farms will increase, quantitative tools are required to predict the air emissions of livestock operation systems at farm and regional scales.

During the past two decades, field campaigns were launched to quantify GHG and NH₃ emissions from livestock operations (e.g., Phetteplace et al. 2001; Jungbluth et al. 2001; Harper et al. 2004). Measurement programs are essential but expensive and thus have not been extensively implemented. Constant emission factors have long been utilized for quantifying the manure-induced gas emissions (Ad Hoc Committee on Air Emissions from Animal Feeding Operation et al. 2003; EPA 2004). However, using constant emission factors has proven insufficient for quantifying the gas emissions from livestock housing, manure storage, or manure/fertilizer application on fields. Accurate assessment of air emissions from animal farms with emission factors has not been successful due to the high variability in quality and quantity of the animal waste and the numerous

environmental factors affecting the conversion of the manure to gases across the farm component facilities. Therefore, simulation models that incorporate mass balance constraints are needed to extrapolate air emissions in both space and time (NRC 2003).

During the past two decades, various models were developed to assist estimation of GHG and NH₃ emissions from livestock farms (e.g., Olesen et al. 2006; Schils et al. 2005). Zhang et al. (1994), Harper et al. (2004), Cortus et al. (2007) and De Visscher et al. (2002) developed models to predict NH₃ emission from lagoons based on ammonium concentration, pH, temperature and wind speed at the facility. Farm-scale GHG emission models have been reported by Rotz et al. (2010), Phetteplace et al. (2001) and Mangino et al. (2007). These models were constructed by means of a variety of methodologies including emission factors, empirical equations, and process-oriented mechanisms. Table 1 provides a list of published models with their modeling scopes and methods. Most of these models do not represent farm systems with the mechanistic detail of simulating biogeochemical processes. Since air emissions from livestock operations essentially result from a series of microbial activities, microbe-mediated, biogeochemical process models are the best suited to predicting the formation and emission of gaseous compounds from manure. This paper documents the development of a process-based model that incorporates a matrix of biogeochemical reactions into a computable framework representing the manure life cycle on livestock farms.

Biogeochemical reactions resulting in GHG and NH₃ emissions

Three major GHGs, carbon dioxide (CO₂), nitrous oxide (N₂O) and methane (CH₄), are byproducts of microbial survival in ecosystems (Li 2007). These gases can be produced any place where organic matter and microbes co-exist. From the point of view of biogeochemistry, manure is a complex of organic matter containing minor minerals. As soon as the manure is excreted by the animals, it undergoes a series of reactions such as decomposition, hydrolysis, nitrification, denitrification, fermentation etc., from which the three GHGs as well as ammonia (NH₃) can be produced. Most of the reactions are well documented with detailed mechanisms described through

Table 1 Selected models for quantifying GHG and NH₃ emissions from livestock manure systems

Model ^b	Enteric source			Housing			Compost or heap			Lagoon or tank			Anaerobic digester			Cropland or pasture					
	CH ₄	N ₂ O		CO ₂	CH ₄	N ₂ O	NH ₃	CO ₂	CH ₄	N ₂ O	NH ₃	CO ₂	CH ₄	N ₂ O	NH ₃	CO ₂	CH ₄	N ₂ O	NH ₃	N leach ^a	
ACES			●																		
CEFM	○																				
CONCEPT			●																		
DairyGHG																					
FARMIN																					
FarmGHG																					
Manure-DNDC																					
TwoFilm																					

○ Empirical or emission factor method, ● process-based method

^a N leaching loss is used to calculate indirect N₂O emissions

^b Information sources of listed models: FARMIN: Van Evert et al. (2003), Schils et al. (2005); FarmGHG: Olesen et al. (2006), for cows and heifers; TwoFilm: De Visscher et al. (2002); CEFM: Mangino et al.; Dairy GHG: Rotz et al. (2010); CONCEPT: Zhang et al. (2005); ACES: Cortus et al. (2007)

the classical laws in physics, chemistry or biology. Although these reactions are microbe-mediated, they, as most processes occurring on the planet, are inherently controlled by the principles of chemical thermodynamics and kinetics. It means these reactions are unexceptionally controlled by a group of environmental factors such as temperature, moisture, redox potential, pH, substrate concentration gradient, etc. In theory, the reaction rates can be calculated based on the values of the controlling environmental factors. The quantitative relations among the reactions, the environmental factors and the gas productions have been developed in an existing model, Denitrification-Decomposition or DNDC, which describes the soil organic matter turnover and gas emission processes (Li et al. 1992; Li 2000, 2011). In consideration of similarities between the manure organic matter (MOM) and the soil organic matter (SOM), the biogeochemical processes of SOM developed in DNDC have been fully adopted in the study to describe the MOM turnover in the new model, Manure-DNDC.

Characterization of manure organic matter

The biogeochemical processes describing SOM turnover in DNDC have been intensively tested against datasets of soil organic carbon (SOC) dynamics or GHG fluxes observed worldwide with encouraging results (Giltrap et al. 2010). The original DNDC model simulates SOM turnover based on its quantity and quality (Li et al. 1994). To enable the biogeochemical reactions to be applicable for the MOM generated in livestock operation systems, we must have the MOM characterized at first.

During its life cycle on the farm, the manure continuously undergoes a series of biochemical or geochemical reactions that lead to continuous changes in its quantity and quality (i.e., nutrient constituents). However, at the very beginning of the manure life cycle, the fresh animal waste can be characterized with its primary components, the feces and urine. Fecal material contains a wide spectrum of organic compounds such as undigested litter, living microorganisms, carbohydrates, proteins, fatty acids, celluloses, hemicelluloses and lignin (Clark et al. 2005; ASAE American Society of Agricultural Engineers 2003). When the fresh feces are exposed to aerobic conditions, they immediately start decomposing although

their different components proceed at different rates. It would be ideal to characterize the feces based on their chemical compounds. However, collecting this information is costly and time consuming. To make the manure characterization more feasible for modeling, we simply adopted an approach where the organic matter is partitioned into several sub-pools with different specific decomposition rates. This approach has been utilized in a number of soil models including DNDC to simulate SOM dynamics with promising results (Prescott 1996; Li et al. 1992; Parton et al. 1988).

In DNDC, SOM storage consists of four organic pools namely residual litter, living microbes, humads (i.e., active humus) and passive humus (Li et al. 1992, 1994). The litter pool represents residual litter; the humads pool contains carbohydrates, protein, lipids and other readily decomposable compounds; and the humus pool is resistant compounds with relatively deep humification. Each of the pools has two or three sub-pools with specific C/N ratios and specific decomposition rates (Table 2). In general, the SOM with higher C/N ratios will consist of a larger fraction of resistant litter. Using this approach, Manure-DNDC partitions fresh feces into residual litter, microbial and humads sub-pools based on the C and N contents in the bulk feces (Eq. 1 in Appendix 1). Fresh urine mainly contains urea and other water-soluble nitrogenous compounds. In Manure-DNDC, all the urine N is assumed to be in the form of urea. Table 3 summarizes

Table 2 Manure organic matter pools with default C/N ratios and specific decomposition rates defined in the Manure-DNDC model

Pool name	C/N ratio	Specific decomposition rate (1/day)
Very labile litter	2.35 ^a	0.074 ^a
Labile litter	20 ^a	0.074 ^a
Resistant litter	100 ^a	0.02 ^a
Labile micro-biomass	10 ^c	0.33 ^b
Resistant micro-biomass	10 ^c	0.04 ^b
Labile humads	10 ^d	0.16 ^b
Resistant humads	10 ^d	0.006 ^b
Passive humus	10	0.0001

^a Gilmour et al. (1985)

^b Molina et al. (1983)

^c Knapp et al. (1983)

^d Stevenson (1982)

the C, N and water contents in the fresh wastes of various animals based on literature. When bedding with sawdust, straw or other organic solids is applied, the fresh animal waste is mixed with the bedding materials to compose the fresh bulk manure. It is the initial step for modeling manure turnover to partition the fresh manure into the various organic sub-pools.

Decomposition

Decomposition is a microbe-mediated process leading to degradation or mineralization of organic compounds in the manure. When the manure is excreted from the anaerobic digestive systems in animal, it is exposed to oxygen and other chemical agents that lead instantly to decomposition of the organic compounds existing in the manure. The microbial decomposers that live in the organic matter utilize available carbon as an energy source and respire CO₂. During decomposition, the labile part of manure will be consumed first leaving the more resistant C in the residue manure. Manure-DNDC simulates manure decomposition by simultaneously calculating the decomposition rates for all the manure sub-pools. Figure 1 shows the sequential decomposition processes embedded in DNDC and now inherited in Manure-DNDC, which convert the manure litter to microbial biomass, humads, and finally humus. During the decomposition processes, each sub-pool decomposes independently following the first-order kinetics (see Eq. 2 in Appendix 1). As a microbe-mediated process, the rate of decomposition is subject to temperature and moisture. The decomposition rate declines if the environmental temperature or moisture content deviates from its optimum (Molina et al. 1983; Stanford and Smith 1972; Smith et al. 1980; Deans et al. 1983, 1986; El-Haris et al. 1983). Because the aerobic decomposition requires oxygen as an electron acceptor, improvement of aeration in the farm facilities accelerates the decomposition rate. However, decomposition can also take place under anaerobic conditions where hydrolysis degrades carbohydrates, proteins, celluloses and even lignin, especially when accompanied by high temperature or catalyzing microbes. The degradation of manure in anaerobic digesters is an example of enhanced anaerobic decomposition. During decomposition, the organic N co-existing with the organic C in the manure is mineralized to ammonium (NH₄⁺), an inorganic ion commonly found in the

Table 3 Default water content, C/N ratio and urine N content in fresh animal wastes

Animal	Urine production, kg/head/day	Water fraction in feces, w/w	Urine N fraction of total waste N, w/w	C/N ratio in feces	C/N ratio in urine
Dairy cattle	10.0	0.8	0.5	16.0	1.25
Beef	10.0	0.8	0.5	16.0	1.25
Veal	10.0	0.8	0.5	16.0	1.25
Pig	3.3	0.82	0.79	18.5	4.24
Sheep	0	0.68	0	3.1	–
Poultry	0	0.8	0	7.9	–

Sources: Ad Hoc Committee on Air Emissions from Animal Feeding Operation et al. (2003), Harper et al. (2004), Jongbloed and Lenis (1998), Cook (2000), Chadwick et al. (2000)

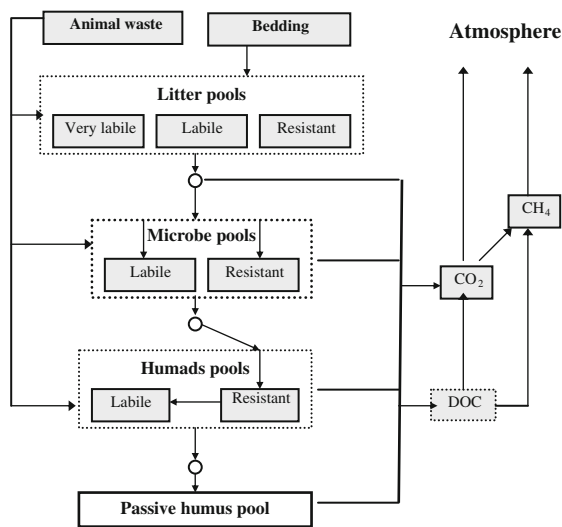


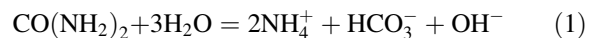
Fig. 1 In Manure-DNDC, the manure carbon (C) consists of four major C pools including litter, microbes, humads and humus with specific decomposition rates and C/N ratio values

manure across the livestock farm facilities (Powell et al. 2006; Pell 2006). The above-summarized decomposing processes are applied in Manure-DNDC to simulate the manure turnover in feedlot, compost, lagoon, anaerobic digester or cropping field soil of the modeled livestock farms.

Urea hydrolysis

Hydrolysis is a reaction converting urea into NH_4^+ that has been commonly observed across all the farm facilities. In this chemical reaction, a water molecule is split into hydrogen and hydroxide ions, and then readily reacts with urea. During the hydrolysis of urea, a molecule of urea ($\text{CO}(\text{NH}_2)_2$) is converted to two

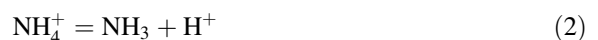
molecules of NH_4^+ with a hydroxyl (OH^-) released (Eq. 1).



Hydrolysis of urea is catalyzed by urease, an enzyme whose activity is subject to temperature, moisture, and available organic carbon components (Schwab and Murdock 2005). In Manure-DNDC, the urease activity in manure is calculated as a linear function of temperature, moisture and dissolved organic carbon (DOC) content, and the urea hydrolysis rate is a first order function of the urease activity and the urea concentration (see Eqs. 3 and 4 in Appendix 1). The importance of urea hydrolysis for manure biogeochemistry is due to not only its conversion but also effects on the environmental pH. As shown in Eq. 1, hydrolysis of urea elevates the pH due to the hydroxyl release that hence affects a series of biogeochemical reactions, especially for NH_3 volatilization. Urea hydrolysis can take place in the manure wherever the relevant substrates are available and the environmental factors are favorable. As this process can occur rapidly, high NH_3 emissions are usually observed in the housing or feedlot facility, the first stage of the manure life cycle.

Ammonia volatilization

When NH_4^+ is produced from either MOM decomposition or urea hydrolysis, the NH_4^+ dissolved in the manure liquid will rapidly reach into equilibrium with the dissolved ammonia (NH_3) (Eq. 2).

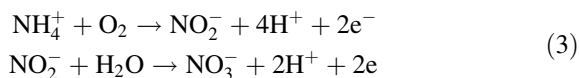


This chemical reaction can occur in either direction depending on the concentrations of NH_4^+ , NH_3

and H^+ in the liquid phase. To determine the direction and the rate of the reaction, two dissociation constants for the NH_4^+/NH_3 equilibrium (K_a) and the H^+/OH^- equilibrium (K_w), respectively, are utilized to calculate the chemical reaction kinetics. As K_a or K_w is temperature-dependent, Manure-DNDC calculates K_a or K_w as a function of temperature (Eq. 5 in Appendix 1) following the work of Glasstone (1946), Sutton (1990) and Sutton et al. (1993). As soon as NH_3 is formed in the manure liquid, it can diffuse to the liquid/air interface driven by the NH_3 concentration gradient in the liquid phase. A two-film model is used in Manure-DNDC to predict NH_3 emission from the manure liquid surface into the air. Following De Visscher et al. (2002), the Henry's law and NH_3 mass transfer coefficients are used to support the two-film model in Manure-DNDC (Eq. 6a–c in Appendix 1).

Nitrification

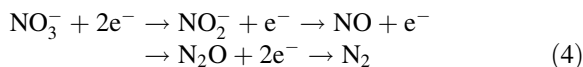
Under aerobic conditions, NH_4^+ can be oxidized to NO_2^- and further to NO_3^- by microbial ammonium oxidizers (i.e., nitrifiers) (Eq. 7 in Appendix 1) (McGill et al. 1981; Van Veen and Frissel 1979). This two-step process is called nitrification (Eq. 3).



As a microbe-mediate process, the rate of nitrification is regulated by the Michaelis–Menten equation, in which the nitrifiers' activity relies on two substrates, DOC and NH_4^+ . Based on Blagodatky and Richter (1998), the growth and death rates on nitrifiers are set as functions of DOC and temperature. The reaction rate is also subject to other environmental factors such as moisture, Eh and pH (Watts and Hanks 1978; Hadas et al. 1986). For example, pH could affect nitrification rate by changing the urea hydrolysis or NH_3 volatilization loss rate in the manure systems. During the process, byproduct NO or N_2O can be produced at a rate proportional to the bulk nitrification rate (Bremner and Blackmer 1978; Parton et al. 1988). Based on Bremner and Blackmer (1981), the nitrification-derived N_2O is a fraction of the nitrification rate, but this fraction is set as a function of temperature and moisture in Manure-DNDC.

Denitrification

Denitrification is a series of microbe-mediated reactions that sequentially reduce nitrate (NO_3^-) to nitrite (NO_2^-), nitric oxide (NO), nitrous oxide (N_2O), and finally dinitrogen (N_2). As reductive reactions, the denitrifying sequence can occur only under anaerobic conditions.



Leffelaar and Wessel (1988) presented a detailed description of denitrification processes based on lab incubations with soil samples. They observed that the rate of each step of the sequential reactions depended on the concentration of the corresponding nitrogenous oxides (i.e., NO_3^- , NO_2^- , NO, or N_2O), and all the reactions competed for available C (i.e., DOC). These relationships were applied in Manure-DNDC to form the denitrification algorithms.

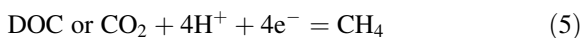
In Manure-DNDC, conditions for denitrification occur if the environmental Eh drops lower than 650 mV, which implies that the anaerobic microsites start forming in the manure (“Eh” below explains how the environmental Eh is calculated). The denitrifiers grow by consuming the corresponding nitrogenous oxides; and the growth rates are taken to be proportional to their respective biomass (van Veen and Frissel 1979; see Eq. 8a in Appendix 1). The relative growth rates of denitrifiers are calculated with the dual-nutrient-dependent Michaelis–Menten equation (Bader 1978). Following Leffelaar and Wessel (1988), we assume that the relative growth rates for denitrifiers are independent of the nitrogenous oxide substrates but that they compete for the common DOC substrate (Eq. 8c in Appendix 1). The denitrifier death rate is a constant fraction of the denitrifier biomass (Eq. 8b in Appendix 1). The dead denitrifiers are added to the humads pool and no longer participate in the dynamic processes.

The effects of soil pH and temperature on denitrification have been incorporated in Manure-DNDC based on observations reported by a number of researchers (Mueller et al. 1980; Klemedtsoon et al. 1978; Burford and Bremner 1975; Stanford et al. 1975a, b; Khan and Moore 1968; Wijler and Delwiche 1954; Focht 1974; Leffelaar and Wessel 1988; Nommik 1956; Dawson and Murphy 1972; Bailey and Beauchamp 1973; Knowles 1981; Keeney et al. 1979;

Bremner and Shaw 1958) (Eq. 8a in Appendix 1). DOC is used by denitrifiers as the basic material for cell synthesis and energy (Pirt 1965). The consumption rate of DOC depends on the denitrifier biomass, relative growth rate, and the maintenance coefficients of the denitrifier populations (Eq. 8c in Appendix 1). According to Leffelaar and Wessel (1988), the maintenance coefficients must be multiplied by the relative presence of each electron acceptor in the water phase (Eq. 8d in Appendix 1). Based on the growth rates of denitrifiers and the C/N ratio in the bacteria, the assimilation of N during denitrification is calculated (Eq. 8e in Appendix 1). A C/N ratio (by weight) of 3.45 is used based on the chemical composition of the denitrifiers ($C_6H_{10.8}N_{1.5}O_{2.9}$), in accordance with data reported for *Paracoccus denitrificans* (van Verseveld and Stouthamer 1978). CO_2 production from denitrification is calculated as the difference between the total amount of consumed C and the amount used for cell synthesis.

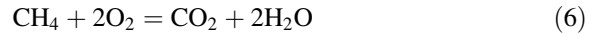
Fermentation

If manure is under anaerobic conditions for a relatively long-term (e.g., several days or weeks), the oxidants such as oxygen, nitrate, 4-valent manganese (Mn^{4+}), 3-valent iron (Fe^{3+}) and sulfate in the manure could be depleted by the decomposers, denitrifiers, manganese bacteria, iron bacteria and sulfur bacteria, respectively. When this occurs, a low Eh (< -200 mV) status develops in the manure, which stimulates another group of microbes that thrive under anaerobic conditions. These anaerobic microbes gain energy by breaking down the organic polymers (e.g., carbohydrates, proteins, fats) into their smaller constituent parts such as sugars, amino acids or fatty acids. The sugars and amino acids can then be utilized by the acidogenic bacteria to produce CO_2 , hydrogen (H_2) and organic acids. Finally, methanogens convert these products to CH_4 by using the C in DOC or CO_2 as electron acceptors (Eq. 5).



Methane production with organic matter is a biochemical process controlled by both physiochemical and biological factors (Crill et al. 1988; Conrad 1989). The activity of methanogens is sensitive to the environmental Eh, pH and temperature. These three factors as along with the concentrations of DOC and

CO_2 are used as drivers to quantify CH_4 production in Manure-DNDC (Eq. 9a in Appendix 1). The CH_4 produced under the anaerobic conditions is vulnerable in the relatively high Eh environment (> -100 mV). When the CH_4 produced at the anaerobic microsites diffuses into the aerobic microsites, the CH_4 oxidizes (Schipper and Reddy 1996; Wang et al. 1993; Kludze et al. 1993):



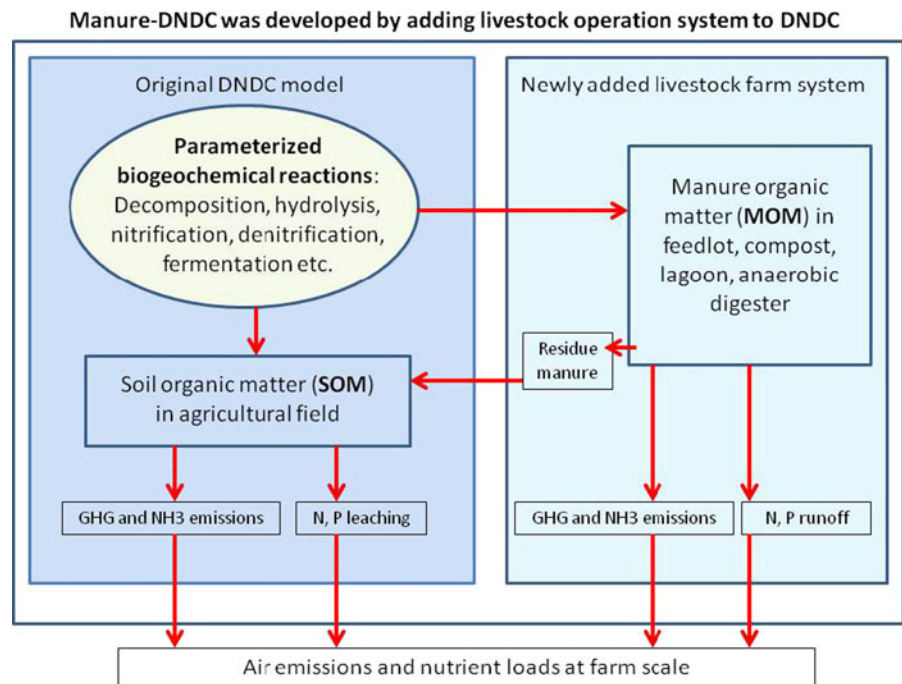
In Manure-DNDC, CH_4 oxidation rate is calculated based on CH_4 concentration and manure Eh (Eq. 9b in Appendix 1). A simplified equation was adopted in Manure-DNDC to estimate CH_4 diffusion within the manure based on the CH_4 concentration gradient, temperature and air-filled porosity (Eq. 9c in Appendix 1). As the methanogenesis processes rely on low Eh and C sources, altering either of these factors could effectively mitigate CH_4 production in the manure.

During the past two decades, the above-described biogeochemical reactions parameterized in DNDC have been widely tested against SOM dynamics in and GHG emissions from agricultural soils observed worldwide. In the development of Manure-DNDC, all the biogeochemical processes embedded in DNDC were inherited in the new model framework by linking them to the manure life cycle across the feedlot, compost, lagoon, anaerobic digester and field application at the farm scale. Figure 2 illustrates how the new Manure-DNDC model overlaps with the original DNDC model by sharing the parameterized biogeochemical processes. The linkage of the biogeochemical processes to the manure life cycle was realized by (1) constructing a new modeling framework that tracks the manure life cycle across the farm component facilities (e.g., feedlot, manure storage/treatment, field application) and (2) modeling the environmental variations in each of the farm components to drive the biogeochemical reactions occurring in the component.

Enteric gas emissions

Methane production from enteric fermentation in rumen animals is a major source of greenhouse gas emission from livestock systems. Empirical or mechanical models were developed by the Intergovernmental Panel for Climate Change (IPCC) and a number of researchers for prediction of CH_4 emissions from the rumen animals (Gibbs and Leng 1993; Schils

Fig. 2 Manure-DNDC was developed by linking the biogeochemical reactions existing in the original DNDC model to the manure life cycle across livestock farm facilities including feedlot, compost, lagoon and anaerobic digester. The gas emissions as well as nutrient loading from both the livestock operation system and the cropping field constitute the farm-scale environmental contributions



et al. 2005; Wilkerson et al. 1995; Monteny et al. 2001). Because the current version of Manure-DNDC has no nutrition module yet, an empirical approach was used to predict rumen CH₄ production based on the IPCC method (IPCC, 1992) as well as the experimental data measured by Mitloehner and his colleagues (Shaw et al. 2007; Sun et al. 2008; Mitloehner et al. 2009; Hamilton et al. 2010) through relevant projects. Fixed methane conversion factors were set as 17.1 and 6.5 % of gross energy demand for dairy cow and beef or veal, respectively (Eq. 10 in Appendix 1). There are very few reports on enteric production of N₂O. Velthof and Oenema (1997) reported that 0.005 % of intake N could contribute to enteric N₂O emission. However, our chamber experiments indicate a higher rate of enteric N₂O (0.2 %) emission from dairy cows. Based on our observed data, an equation was used in Manure-DNDC to estimate enteric N₂O flux as a linear function of the daily N intake (Eq. 11 in Appendix 1).

Manure life cycle across farm facilities

The framework of Manure-DNDC was developed based on the manure life cycle within the farm scale.

Livestock farms in the U.S. usually include three major component facilities: feedlot, manure storage/treatment facilities and field application. The feedlot facility can include barns or outdoor corrals. The manure treatment/storage facilities include lagoon, tank, compost and anaerobic digester. For most farms, the manure is produced in the feedlot, then moved to the storage or treatment facilities, and finally applied to the cropping field. If the crop harvested from the field is used as forage to feed the animals on the farm, the manure nutrient cycle is closed at the farm scale. During its movement through the farm component facilities, the manure experiences different environmental conditions usually characterized with the temperature, moisture, Eh, pH and substrate concentration in the facilities. These environmental factors drive the biogeochemical reactions occurring within the manure, and hence continuously change its amount and chemical composition. GHG and NH₃ fluxes from each component result from the biogeochemical reactions in the component. Figure 3 illustrates how Manure-DNDC integrates the farm components, the biogeochemical reactions and the gas emissions into a modeling framework. Users can select the candidate components and then link them in parallel or series to construct a virtual farm that mirrors their actual farm.

Manure-DNDC Modeled C, N and P Biogeochemical Cycles in Livestock Farms (Red lines represent mass flow, and blue lines information flow)

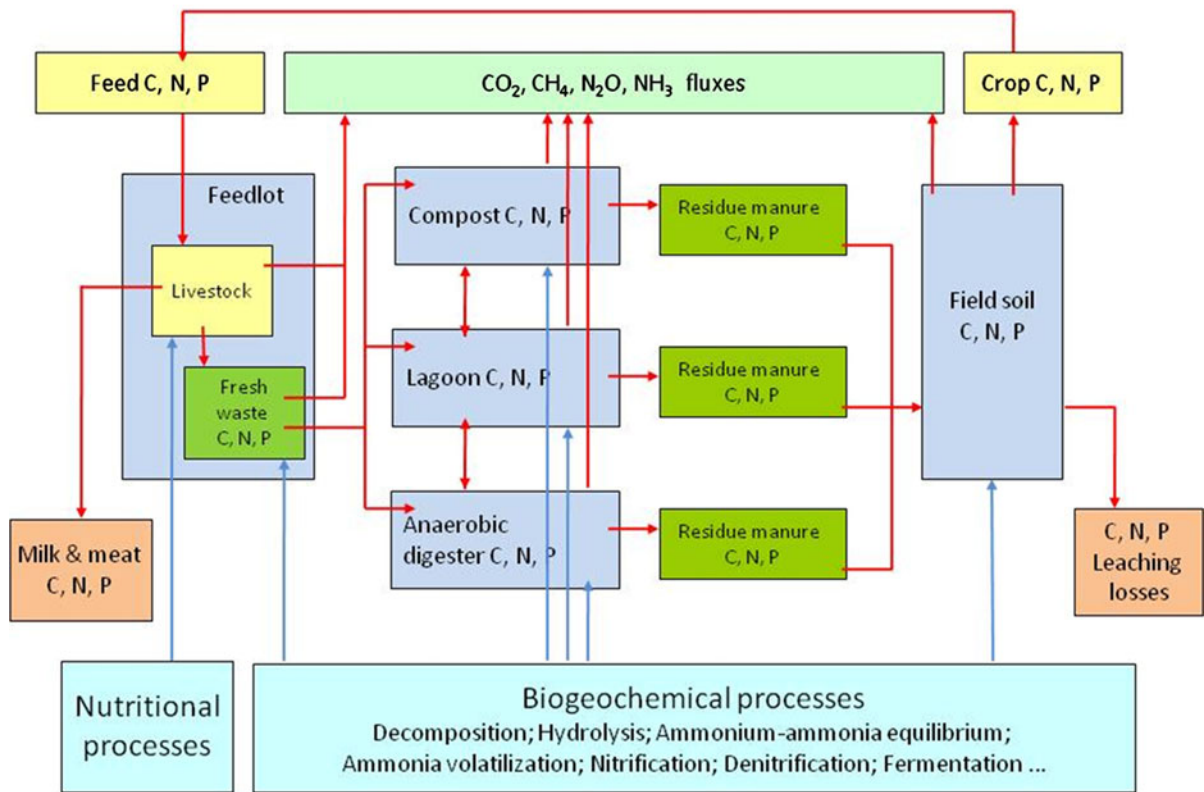


Fig. 3 In Manure-DNDC, feeding lot, compost, lagoon, anaerobic digester and crop field are integrated by tracking C, N and P cycles across the farm component facilities, from which CO_2 , CH_4 , N_2O or NH_3 is produced. In the figure, and the blue arrows represent impacts of the biogeochemical processes on

the quantity and quality of the manure in the corresponding farm facilities. The nutrient cycles will be closed if the forage produced from the crop field is used as the feed for the farm stock. (Color figure online)

Seven candidate farm components have been parameterized in Manure-DNDC. Their functions and technical specifications are described as follows.

Manure production

The manure life cycle begins with animal excretion. Animal excretion rate depends on a number of factors such as animal breed, age, weight, health, production level, amount and type of feed etc. (Kulling et al. 2003; Oenema et al. 2005). Manure-DNDC defines the quantity and nutrient content of fresh animal waste based on the livestock type, feed rate and crude protein content in feed. Manure-DNDC can represent six types of animals, i.e., dairy cows, beef cows, veal calves, swine, sheep and poultry. Feed rate (in kg dry matter/head per day) and crude protein (CP)

concentration (%) in feed are required as input data. About two hundred of feed materials commonly used on U.S. farms have been included in a library file in Manure-DNDC to allow users to compose their feeds. The generalized contents of dry matter, CP and phosphorous (P) in each feed material are adopted from Subcommittee on Dairy Cattle Nutrition and Committee on Animal Nutrition (2001) and Maiga et al. (1997). Manure-DNDC calculates the dry matter, CP and P contents based on the user-selected combinations (Appendix 2).

In Manure-DNDC, fresh animal manure is characterized by its C, N, P and water content, which are calculated based on the input information of animal type, population and diet. The C content in the feed is a constant fraction (40 %) of the feed dry matter; and the N content in the feed is calculated based on the feed

CP concentration (1 kg N per 6.25 kg CP). The manure C content is the difference between the total amount of feed C and the C losses through animal respiration, weight gain and milk production (Ad Hoc Committee on Air Emissions from Animal Feeding Operation et al. 2003). The manure N content is the difference between the total N intake and the N secreted in milk and meat. Following Powell et al. (2006), we assumed 25 % of the CP fed to dairy cows was secreted in milk in the model.

Manure in feedlot facility

Manure begins its life cycle following excretion in the feedlot facility. Based on the descriptions of the U.S. cattle housing facilities by Miller and Berry (2005), Manure-DNDC defines the facility by its ground surface area, surface property (e.g., solid concrete or slatted floor), sheltering and ventilation. Manure-DNDC differentiates outdoor pen from barn based on the defined conditions of sheltering and ventilation. The barn has a shelter and hence the indoor temperature or moisture is more or less different from the weather conditions. Two types of floor, i.e., solid concrete and slatted with a below-ground gutter, can be used. Both the solid and liquid wastes can fall into the gutter although with the user-defined portions. Using the slatted floor will separate the manure liquids from the solids. The separating proportions are defined by the user. The outdoor pen can have a concrete floor or a bare soil surface, which affects the leaching loss of N or P. The manure stored in the barn or outdoor pen is removed at a defined frequency. When the manure is removed from the feedlot, the users will need to specify the proportions of the liquids and solids transported to the compost, lagoon and/or anaerobic digester.

The manure accumulated on the feedlot floor undergoes decomposition, hydrolysis, nitrification, denitrification, ammonia volatilization, fermentation and other biogeochemical reactions under the feedlot environmental conditions (e.g., temperature, moisture, Eh, pH etc.). Through these processes, the quantity and nutrient composition of the manure are changed. Manure-DNDC tracks the changes in the manure's quantity and quality in the feedlot facility and passes the residue manure to the next component (e.g., compost, lagoon or anaerobic digester) of the manure life cycle. Simulating the biogeochemical reactions,

Manure-DNDC calculates emissions of CO₂, CH₄, N₂O and NH₃ from the feedlots.

Manure storage/treatment

The manure removed from feedlot can be placed into compost, lagoon or anaerobic digester facility for storage or treatment. During the storage or treatment, the manure undergoes the same series of biogeochemical reactions although under different environmental conditions. The processes further change the quantity and nutrient constituents of the manure. The three optional storage/treatment facilities differ in their technical specifications and hence possess different environmental conditions to affect the manure fate.

In Manure-DNDC, compost is defined by its density, storage duration, aeration and additives. In compost, the manure solids decompose at a rate determined by the nutrient contents of the manure as well as the compost climate (e.g., temperature, moisture, aeration, etc.). During the decomposition, the most labile organic C in the manure is first converted into CO₂ meanwhile the corresponding part of the organic N transformed to inorganic N (i.e., NH₄⁺ and NO₃⁻). The process generates heat to elevate temperature in the compost. N₂O can be produced through either nitrification or denitrification during composting (Brown et al. 2000; Hao et al. 2004, 2005; Pattey et al. 2005). If part of the compost is very moist, CH₄ could be produced through fermentation; however, the high redox potential at the surface of the compost could oxidize a large fraction of the CH₄ produced within the facility (Peterson et al. 2005). Through nitrification and ammonium/ammonia equilibrium, NH₃ gas can be produced and emitted from the compost. Manure-DNDC tracks changes in the manure quantity and quality by simulating all the biogeochemical reactions occurring during composting.

A lagoon or slurry tank receives the manure liquids for storage and treatment. In Manure-DNDC, a lagoon is characterized by its capacity, surface area, coverage, and retention time (Hatfield et al. 1993; Doorn et al. 2002; Harper et al. 2004). When the slurry manure is stored in a lagoon, the aerobic decomposition process will be depressed while urea hydrolysis, NH₄⁺/NH₃ transformation and fermentation will be enhanced to produce CH₄ and NH₃. Under the anaerobic conditions, production of nitrate through nitrification is

usually depressed, which consequently reduces denitrification rate in the lagoon. However, if the influx of manure contains a high concentration of nitrate, the denitrification process could be highly stimulated to convert the nitrate to N gases (e.g., N_2O , N_2). Manure-DNDC simulates the gases produced in and emitted from the slurry manure with wind speed affecting the processes (Amon et al. 2004). If the content of solids in a lagoon or slurry tank is high, a crust can form along with the loss of the moisture in the liquid storage that will alter the Eh and temperature of the manure and hence affect a series of biogeochemical processes including nitrification, denitrification, NH_3 volatilization and fermentation occurring in the manure.

An anaerobic digester is an engineering facility designed with operating conditions of temperature, retention time, pH and feedstock quantity and quality to promote the anaerobic digestion (Weiske et al. 2006; Zhang et al. 2004, 2005; Alvares and Liden 2008). In Manure-DNDC, the digester is modeled as an anaerobic reactor with a continuous feedstock flow. The influx rate or frequency is determined by the upstream manure removal. The anaerobic decomposition occurring in the digester is dominated by hydrolysis, which converts a wide range of organic matter (from carbohydrates to lignin) to DOC (or organic acids), which fuels the methanogens in the digester. This process is temperature-sensitive. In Manure-DNDC, we assume the microbial catalyzer is in optimum status, and hence the temperature and chemical constituents of the manure are the major controls for the fermentation processes occurring in the digester. While the manure organic C transforms to DOC, CO_2 or CH_4 , the organic N transforms to NH_4^+ . The NH_4^+ will remain in the residue slurry due to the depressed nitrification. By simulating the hydrolysis and fermentation processes, Manure-DNDC calculates CH_4 production as well as alters the nutrient constituents of the treated manure.

Manure-DNDC allows the manure to be transported between the three treatment facilities (i.e., compost, lagoon and anaerobic digester) and hence enable the users to integrate the components in parallel or series to mimic the actual manure flow path in their farms.

Manure field application

Most dairy farms in the U.S. possess crop fields or pastures, where manure can be land applied while

producing forage and other feeds. The manure field application process usually has a dual purpose that uses the manure as fertilizer for crop production and the field for disposal (Sharp et al. 2004). Manure application to a field enhances air emissions as well as nutrient runoff or leaching losses that result in a series of environmental issues (McGechan and Lewis 2000; McGechan and Topp 2004; Lewis et al. 2003). The environmental consequences depend on the residue manure constituents, the climate conditions, the soil properties, and the cropping management regime on the farm.

In Manure-DNDC, the field receiving the residue manure can be a cropland or a pasture. If it is a cropland, it will be defined by its total area, crop type/rotation, and cropping management practices (e.g., tillage, fertilization, manure application method, irrigation etc.). About fifty crops commonly planted in the U.S. have been parameterized in Manure-DNDC based on their statistics of yield, biomass partition, C/N ratio and other physiological or phenology properties. Manure-DNDC precisely simulates the crop growth to determine its demands for water, N and P, which will be further used to calculate the water, N and P uptake from the soil. Based on the modeled temperature, water or nutrient stress, Manure-DNDC predicts the crop yield as well as the biomass partitioning to grain, shoot and roots. After harvest, the crop residue is partially or totally incorporated back into the soil to affect the soil C, N and P dynamics. The frequency of manure field application is determined by the timetable of manure removal from the upstream farm facilities (e.g., feedlot, compost, lagoon or anaerobic digester), which are defined by the users as part of management practices for the storage/treatment facilities. The information exchange between the storage/treatment facilities and the cropping field is at a daily time step. In Manure-DNDC when the residue manure is removed from the storage or treatment, the manure is characterized with a series of chemical components including litter, microbes, humus, DOC, urea, NH_4^+ , NO_3^- , NH_3 etc. When the manure is incorporated in the field soil, the manure components will be added into the corresponding soil pools to undergo the routine soil biogeochemical processes (e.g., decomposition, hydrolysis, nitrification, denitrification, NH_3 volatilization, fermentation etc.). Since the algorithms describing crop growth and soil biogeochemistry

developed in DNDC have been well documented during the past two decades (see a summary by Giltrap et al. 2010), no details of them are provided in this paper.

If there are several different crops planted in the farm fields that receive the same source of manure, the proportion of the manure applied to each crop field must be specified as input information by the user.

The manure field application can be conducted with two options, surface application or injection. If the modeled crop or forage is used to feed the livestock on the same farm, the manure life cycle will be closed within the farm that provides a basis for evaluating the feed efficiency, fertilizer use efficiency, and manure treatment efficiency at the farm scale.

If the field is used as a pasture, besides defining the field plants, the grazing practices will need to be defined. Based on the user-defined animal type, population and grazing timing and duration, Manure-DNDC calculates the grass consumption and animal waste production at daily time step. The fresh waste is deposited in the field and incorporated in the surface soil. Manure-DNDC partitions the fresh waste into three parts, urine, undigested little and humus, and then adds them into the corresponding soil organic matter pools.

In summary, Manure-DNDC provides candidate farm component facilities for the users to compose their own virtual farm, based on which the users could not only estimate GHG and NH₃ emissions from the farm but also test management alternatives for mitigation.

Environmental factors driving biogeochemical reactions

All the biogeochemical reactions, no matter where they take place, are universally controlled by the principles of thermodynamics and reaction kinetics. The former determines if a reaction can occur, and the later defines its rate when the reaction takes place. The principles regulate the biogeochemical reactions through the collective effects of a group of environmental forces or factors, which include temperature, moisture, pH, Eh and substrate concentration gradient for most ecosystems. These environmental factors constitute a multi-dimensional field, ever varying in space and time, to determine occurrences and rates of

the biogeochemical reactions in ecosystems (Li 2007). In Manure-DNDC, the variations of the environmental factors in each farm component are simulated based on the natural climate/soil conditions, the farm facility specifications, and the management practices. Daily weather data (e.g., air temperature, precipitation, wind speed etc.) and soil properties (e.g., bulk density, texture, SOC content and pH) are used in conjunction with the farm component specifications to track the variations of the environmental factors for each farm component at a daily or hourly time step.

Temperature

Temperature is directly related to the kinetic energy of particles and hence controls almost all chemical reactions. The balance between the influx and efflux energies determines the variation in temperature for any system. Manure-DNDC tracks temperature variation for each farm component with the methods described as follows.

Feedlot. Manure-DNDC simulates three types of feedlots including barn, outdoor pen and pasture. The temperature in barn is calculated based on the ambient outside air temperature but adjusted for the ventilation rate (Eq. 1 in Appendix 3). The soil temperature in the outdoor pen or pasture is set to be identical to the air temperature obtained from the input daily weather data.

Compost. Temperature varies in compost throughout the composting cycle. When the fresh manure, sometimes with additives, is piled to initiate composting, the temperature in the compost increases rapidly due to the heat released from oxidation of the labile organic matter contained in the manure. The increase in temperature accelerates the decomposition processes to eventually exhaust the labile organic matter, which leads to a decrease in heat generation in the compost. Manure-DNDC calculates the heat generation in the compost as well as the heat transfer at the interface between the compost and the air driven by temperature gradients. The change in temperature is calculated based on the heat balance and the heat capacity of the compost (Eq. 2 in Appendix 3).

Lagoon. Temperature varies in a lagoon based on the air temperature, wind speed, lagoon geometry and coverage. The lagoon temperature lags behind the air temperature due to the water heat capacity as well as the water depth. A simplified heat transfer formula is

used in Manure-DNDC to estimate the daily temperature change in lagoon (Eq. 3 in Appendix 3).

Anaerobic digester. Temperature in an anaerobic digester is defined by its technical specifications. In Manure-DNDC, the anaerobic digester is classified by three types based on their optimal temperature ranges, i.e., psychrophilic (<20 °C), mesophilic (30–40 °C) and thermophilic (50–60 °C). Manure-DNDC simulates the anaerobic digester as a continuous flow reactor with a hydraulic retention time defined by the user. The temperature remains constant during the operation.

Field soil. Manure-DNDC calculates a soil temperature profile based on a heat transfer algorithm. In the algorithm, the soil surface temperature, soil heat capacity and soil heat conductivity are calculated for each soil layer to determine the soil temperature profile on a daily time step (see details in Li et al. 1992).

Moisture

Moisture plays a dual role in manure biogeochemistry. Most of the biochemical or geochemical reactions take place only in the liquid phase on one hand; and almost all the microbes survive relying on water availability on the other hand. Manure-DNDC estimates water content in the manure based on the mass balance between the water input and output for each farm component.

Feedlot. Water content of the manure accumulated on the feedlot floor is dynamic driven by the water input to and output from the floor. The influx can come from the excreted urine and feces, flushing solution and precipitation; and the efflux takes place through evaporation, soil infiltration, or manure removal. In manure-DNDC, if the manure solids and liquids are mixed on the floor, the manure moisture is determined as the total of the urine and feces water contents. If the solids and liquids of manure are separated, Manure-DNDC arbitrarily partitions 80 % of the urine and 20 % of the feces to the under-floor gutter with the rest remaining on the floor. However, this default setting can be redefined by users. The slurry stored in the gutter is saturated. Manure-DNDC calculates daily potential evapotranspiration (PET) based on the Penman–Monteith equation (FAO, 2009), and the field PET is adjusted for the housing climate conditions. For example, for the barns with ventilation, the

wind speed is adjusted based on the ventilation rate. For the outdoor pen or grazing plot, the wind speed value is from the daily weather data. Following Sellers' work on peat soils (1965), we assume that actual evaporation of the manure-water decreases linearly with PET to zero as the manure-water potential drops from -0.033 to -1.5 MPa. Manure-DNDC updates the manure moisture at a daily time step.

Compost. The initial water content in compost is the manure moisture plus the water added during the compost formation process. Changes in compost moisture are driven by evaporation and precipitation during the composting period. Manure-DNDC empirically estimates daily evaporation rate based on the compost temperature, density and water content (Eq. 4 in Appendix 3).

Lagoon, tank or anaerobic digester. The manure stored in lagoon, tank or anaerobic digester is assumed to be saturated.

Field soil. Manure-DNDC calculates the vertical and horizontal water movement in the soil based on precipitation, topography and soil hydraulic properties by following the methods established in DNDC (see details in Li et al. 1992; Zhang et al. 2002; Deng et al. 2011). When the manure is incorporated in the field soil, the manure water is added to the soil. Two hydrological methods, SCS and MUSEL functions, have been incorporated in Manure-DNDC to estimate surface runoff and soil erosion at farm or watershed scale (Deng et al. 2011) that has enhanced the capacity of the model for quantifying N or P loading from the farm feedlot or cropping field.

Eh

All reductive-oxidative reactions rely on the electron transfer between chemical agents, which includes the production of CO_2 , N_2O and CH_4 in the soil or manure. Environmental redox potential represented as Eh determines the electron transfer capacity (Stumm and Morgan, 1981). The concept of anaerobic balloon has been inherited in Manure-DNDC to estimate the environmental Eh value. If oxygen exists in the manure or soil system, its Eh value varies between 650 and 0 mV with an anaerobic volumetric fraction in the medium varying between 0 and 1 correspondingly. When the manure or soil is saturated with water, oxygen in the system will be depleted, which

will stimulate different groups of microbes to use other oxidants such as nitrate, Mn^{4+} , Fe^{3+} , sulfate and even C as electron acceptors under the deepened anaerobic conditions (Li 2007). In Manure-DNDC, the bulk Eh of manure or soil is calculated based on the Nernst equation (Eq. 5 in Appendix 3). Oxygen content in the manure or soil is calculated based on air-filled pores and the autotrophic and heterotrophic respiration rates. For the slurry manure stored in lagoon or anaerobic digester, a constant Eh value of -300 mV is used.

pH

Environmental acidity represented as pH determines the proton (H^+) transferring capacity, which affects most biogeochemical reactions involving hydrolysis or hydration. For example, the hydrolysis of urea consumes H^+ and elevates the environmental pH which increases NH_3 volatilization by shifting the $\text{NH}_4^+/\text{NH}_3$ equilibrium. In Manure-DNDC, the initial pH of manure is identical to that of the feces or urine. For example, the initial manure pH values are empirically set as 7.0, 7.0, 8.1, 7.5, 7.0, 6.9, and 6.9 for dairy cow, beef cow, veal, pig, sheep, and poultry, respectively. During the manure storage or treatment, Manure-DNDC tracks the production and consumption of H^+ to recalculate the manure pH across the farm components.

Substrate concentration

Most of the biogeochemical reactions embedded in Manure-DNDC are microbe-mediated processes. Based on the Michaelis–Menten equation, a widely applied formula to describe the kinetics of microbial activity with dual nutrients in biology (Paul and Clark 1989), concentrations of the reactants or substrates involved in the reactions are required to calculate the reaction rates (Eq. 6 in Appendix 3).

For the processes producing CO_2 , N_2O , CH_4 or NH_3 , the major substrates are DOC, NH_4^+ and NO_3^- . Manure-DNDC tracks variations of the substrates by simulating their productions and consumptions in decomposition, hydrolysis, nitrification, denitrification, fermentation etc. In addition to the biogeochemical processes, Manure-DNDC also calculates other sources or sinks of the substrates. For example, Manure-DNDC simulates soil N or C inputs from atmospheric deposition, fertilizer application, plant exudation and other sources, as well as soil N or C

outputs through plant uptake, leaching loss or soil erosion. Figure 4 provides an example to show how Manure-DNDC simulates N substrate concentrations by tracking all the relevant processes potentially occurring in livestock farms.

Model framework based on biogeochemical concepts

Biogeochemistry is a scientific discipline, which defines the interactions between life and its inorganic environment by tracking movement of the chemical elements in ecosystems (Vernadsky 1944; Li 2001). Among the four biogeochemical concepts (i.e., abundance, coupling, cycling and field), the biogeochemical field plays a central role in integrating various factors and processes into an ecosystem. A biogeochemical field is the assemblage of forces which control the elementary movement in ecosystems. The forces or factors usually include gravity, radiation, temperature, moisture, Eh, pH and substrate concentration gradient. These factors construct a multi-dimensional field, which determines a series of biochemical or geochemical processes on one hand, and varies in time and space driven by a few primary drivers such as climate, soil, vegetation and management practices on the other hand. The concepts of biogeochemistry have been adopted in the study to build up the framework of Manure-DNDC.

In Manure-DNDC, two bridges were built up to link three basic components (i.e., farm facilities, environmental factors and biogeochemical reactions) for livestock farms. The first bridge predicts the environmental factors (e.g., temperature, moisture, Eh, pH and substrate concentration) based on the primary drivers (e.g., climate, soil, farm facility specifications, management practices etc.); and the second bridge links the environmental factors to the biogeochemical reactions that shape C, N or P cycling, including GHG and NH_3 emissions, at the farm scale (Fig. 5). Within the Manure-DNDC framework, the primary drivers, the environmental factors, the biogeochemical reactions and the gas emissions are mechanically integrated. Any single change in the primary drivers (e.g., management practice) can simultaneously alter one or more of the environmental factors in the relevant farm component facility (e.g., feedlot, compost, lagoon); and the changes in the

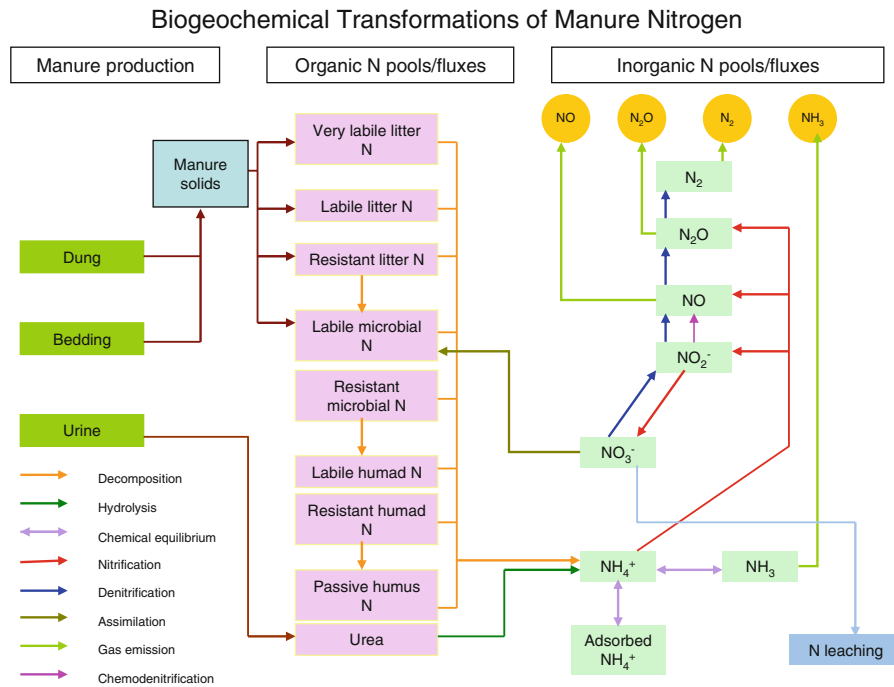
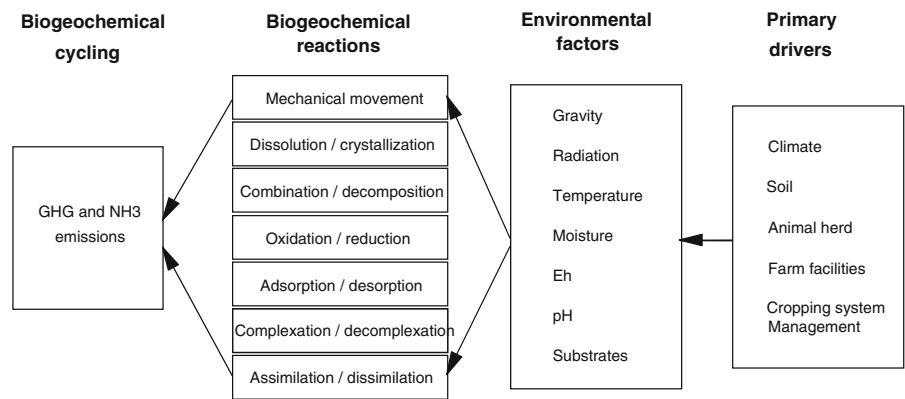


Fig. 4 Nitrogen pools, transport paths and transformations simulated by the Manure-DNDC model

Fig. 5 Manure-DNDC was built upon the biogeochemical concepts, which integrate the primary drivers, environmental factors, biogeochemical reactions and gas emissions into a computable framework



environmental factors can collectively affect several biogeochemical reactions (e.g., decomposition, nitrification, denitrification) that finally affects GHG or NH_3 emissions from the farm. For example, a change in manure application depth can simultaneously alter the soil temperature, moisture, pH, Eh, and concentrations of DOC, NH_4^+ or NO_3^- . These changes will simultaneously and collectively affect the rates of decomposition, nitrification and denitrification occurring in the manure-amended soil that eventually alters the emissions of CO_2 , N_2O and NH_3 from the soil. The correlation between the cause (i.e., a change in

manure application for this example) and the consequence (GHG and NH_3 fluxes) is inherently nonlinear. In addition, the extreme spatial and temporal heterogeneity of many of the primary drivers has obscured the relationship between the causes and effects for many of the biogeochemical processes. Manure-DNDC was developed to handle this complexity.

Manure-DNDC estimates GHG and NH_3 emissions throughout the manure life cycle on a farm by simulating the air emissions from individual farm components (e.g., feedlot, compost, lagoon, anaerobic digester, crop field). The input information required to run Manure-DNDC

Table 4 Input parameters for Manure-DNDC simulation

Category	Description
Climate	Daily weather data: max and min air temperature, precipitation, and wind speed
Stock	Livestock type (dairy cow, beef cow, swine, sheep, poultry) and heads; Feed rate (kg dry matter/had/day) and crude protein and P concentration (%) in feed
Manure storage and treatment	Feedlot: type (barn or outdoor pen), floor conditions (concrete or slatted with under-floor gutter), floor surface area, and ventilation; Bedding: type (sand, manure solids, straw, sawdust etc.); amount (kg dry matter per application), frequency; Manure removal: frequency, fraction of manure removed to lagoon, compost, anaerobic digester or crop field; Compost: density (kg dry matter/cubic meter), storage duration (days), litter additive quantity (kg dry matter) and quality (C/N ratio), fractions of residue manure removed to lagoon, anaerobic digester, or crop field; Lagoon or tank: capacity (cubic m), surface area (square m), coverage (none, loose, tight), retention time (days), fraction of residue slurry removed to anaerobic digester or crop field; Anaerobic digester: processing temperature (psychrophilic, mesophilic, or thermophilic), hydraulic retention time (days), fraction of residue manure removed to lagoon or crop field
Crop field	Crop types (corn, wheat, soybean, alfalfa, sorghum, oats, barley, legume hay, non-legume hay, cover crops, etc.), areas (ha), planting/harvest dates, crop residue management (incorporation or removal), and crop rotations; Tillage: application dates, tilling depth; Fertilization: fertilizer types (urea, anhydrous ammonia, ammonium nitrate, ammonium phosphate etc.), application dates, application rate (kg N/ha), application depth, application method (manual, fertigation or auto-fertilization), use of control-release fertilizer or nitrification inhibitor; Additional manure amendment: date, rate (kg N/ha), quality (C/N ratio), and application method (surface or injection); Irrigation: manual application (based on irrigation events), or auto-irrigation (based on the crop water stress and irrigation index), method (flood, sprinkler or drip); Grass cutting: application dates, cut fraction

includes four categories: livestock herd, farm facility specifications, daily weather data, field soil and management practices. The detailed information of the required input parameters is listed in Table 4. Manure-DNDC simulates on a daily time step for at least 1 year. After the 1-year simulation, the modeled daily and annual pools and fluxes of C, N, P and water are recorded in the result output files. The recorded parameters of C, N, P and water fluxes are summarized in Table 5. Annual fluxes are calculated by summing up the daily results. By reviewing the daily or annual results, the user obtains a relatively complete picture of GHG and NH₃ emissions from the livestock manure system.

Model evaluation tests

Validation against experimental data is an integral part of model development. Field datasets measured on

seven livestock farms in California, New York, North Carolina and Scotland were used to evaluate the model. The datasets covered CO₂, CH₄, N₂O and NH₃ emissions from the freestall barns and drylot corrals, compost, lagoon, and pasture fields. Information for the local climate, soil and farm management of the tested sites were obtained as input parameters to support the model simulations. For each simulation, Manure-DNDC recorded the fluxes of C, N and water from the farm components, which were compared to observations at a daily or annual time step.

Case 1 CO₂, CH₄ and N₂O emissions from a feedlot at University of California at Davis.

Emissions of CO₂, CH₄ and N₂O were measured from a closed feeding cell holding eight beef steers for 14 days in 2007 (Stackhouse et al. 2011). The cell floor had a concrete surface with an area of 100 m². No bedding was applied. The ventilation (i.e., air flow)

Table 5 Daily output parameters produced from Manure-DNDC simulation

Farm component	Output parameters
Livestock	Daily milk production and/or weight gain; Daily production of feces and urine; Daily fluxes of enteric CH ₄ and N ₂ O; Daily fluxes of CO ₂ from animal respiration
Feedlot	Daily fluxes of CH ₄ , N ₂ O, NH ₃ , NO, N ₂ and CO ₂ from floor and/or gutter; Daily removal of feces and urine to compost, lagoon, anaerobic digester or crop field; Daily evaporation
Compost	Daily fluxes of CH ₄ , N ₂ O, NH ₃ , NO, N ₂ and CO ₂ from compost; Daily fluxes of nitrate leached from compost; Daily of organic matter lose with runoff from compost; Daily removal of residue manure from compost to lagoon, anaerobic digester or crop field; Daily evaporation
Lagoon	Daily fluxes of CH ₄ , N ₂ O, NH ₃ , NO, N ₂ and CO ₂ from lagoon; Daily removal of residue slurry manure from lagoon to anaerobic digester or crop field; Daily evaporation
Anaerobic digester	Daily production of CH ₄ , N ₂ O, NH ₃ , NO, N ₂ and CO ₂ from digester; Daily removal of residue manure from digester to lagoon, compost or crop field.
Crop field	Daily fluxes of CH ₄ , N ₂ O, NH ₃ , NO, N ₂ and CO ₂ from field soil; Daily fluxes of nitrate leached from field soil; Daily fluxes of P loss from field soil through runoff; Daily photosynthesis, autotrophic respiration and NPP of crops; Daily N, P and water uptake by crops; Daily soil temperature, moisture, oxygen, pH and Eh profiles; Daily soil ammonium, nitrate and P profiles; Daily soil organic carbon (SOC) profiles; Daily net ecosystem C exchange (i.e., NEE, an indicator of ecosystem C sequestration); Daily transpiration and evaporation

rate was 0.81 cubic m/s. During the experimental period, the feed rate was 15 kg dry matter (DM)/head/day with crude protein (CP) concentration of 13 %; the cell temperature was maintained at 19.5 °C; the feces and urine were mixed with continuous accumulation on the floor of the cell during the experimental period. The manure pH was 8.8. Concentrations of CO₂, CH₄ and N₂O in the influx and efflux air samples were measured continuously and averaged to hourly values. The gas fluxes were calculated based on air flow rates and gas concentrations, and converted to daily fluxes. The observed data indicated that the emission rates of all three gases slightly increased during the 14 day measurement period (Fig. 6).

We simulated the feedlot with Manure-DNDC by setting input parameters consistent with the

experimental conditions. Manure-DNDC modeled daily fluxes of CO₂, CH₄ and N₂O emitted from two sources, i.e., the animal metabolic processes and the manure accumulated on the feedlot surface. The modeled CO₂ fluxes came from animal respiration and manure decomposition; the modeled CH₄ were the sum of the animal enteric CH₄ release and the CH₄ produced in the anaerobic microsites within the manure; and the N₂O came from animal enteric N₂O production and nitrification and denitrification processes in the accumulated manure. Manure-DNDC calculated the manure moisture by tracking the manure water balance between the water input from urine and feces and the output due to evaporation. The modeled fluxes of CO₂, CH₄ or N₂O were generally in agreement with observations regarding the trends and

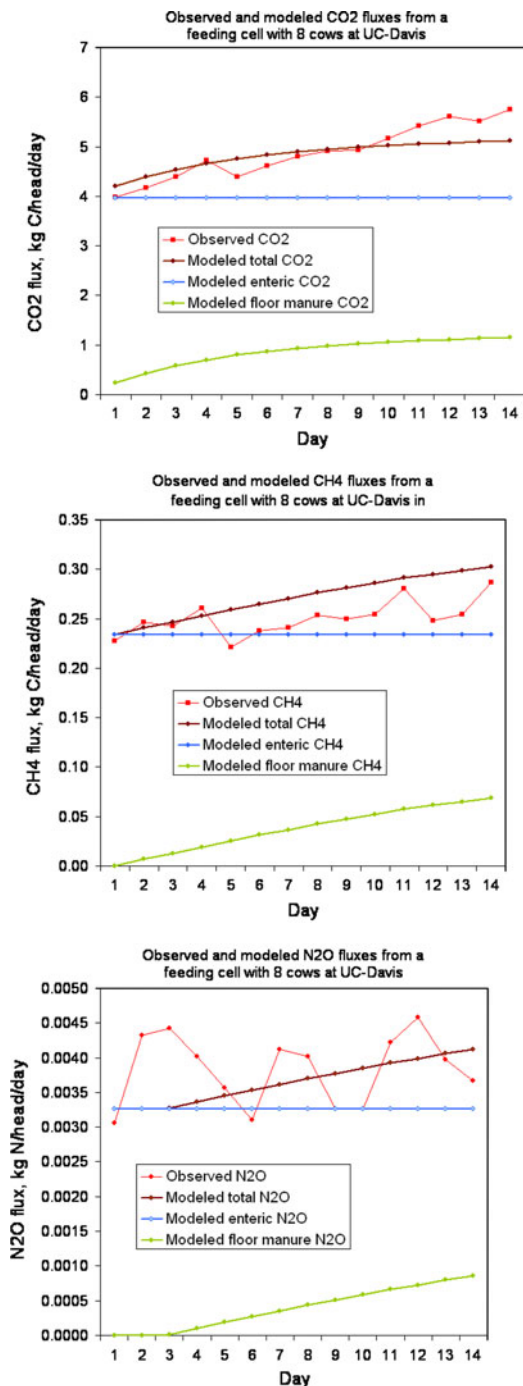


Fig. 6 Comparison between observed and modeled daily CO₂, CH₄ and N₂O fluxes from a closed feeding cell with eight cows in UC-Davis in 2007. The modeled results indicate that the observed variations in the gas fluxes were mainly explained with the air emissions from the manure accumulated in the cell while the respired CO₂ or enteric CH₄ and N₂O emission rates kept constant

magnitudes of the gas fluxes. The modeled results indicated that (1) the animal metabolic sources dominated the fluxes of the three gases with relatively constant emission rates, and (2) the observed increasing trends in the gas fluxes during the experimental period were mainly driven by the manure source, which gradually accumulated on the floor during the experiment (Fig. 6). However, discrepancies existed. For example, the field data showed higher temporal variations, especially for N₂O. The discrepancies could be related to the model assumptions, in which the animal metabolic processes were regarded as constant and the substrate concentrations in the manure were uniform. These assumptions could be inaccurate and thus induce the deviations of the modeled results.

Case 2 NH₃, CH₄, CO₂ and N₂O emissions from a dairy barn in New York.

From November 11, 2007 to October 23, 2009, measurements of NH₃, CH₄, CO₂ and N₂O emissions were conducted in a dairy barn near Skaneateles in New York (Bogan et al. 2010). Concentrations of the gases in the influx and efflux air were measured for the barn. The ventilation rate was 1 cubic m/s. Daily gas fluxes were calculated based on the measured gas concentrations and the air flow rates. During the experimental period, the barn held 470 dairy cows consuming feed containing CP 20 % at the rate of 20 kg DM/day/head. The area of floor was 3,235 m². Straw bedding was used at the rate of 1,070 kg per day. Feces and urine were mixed on the floor, and the slurry was scraped and moved to a lagoon several times per day. The data of the gas fluxes measured in 2008 were used for the validation test.

Daily weather data (i.e., maximum and minimum air temperature, precipitation and wind speed) were obtained from the nearest climate station in Onondaga, NY. Driven by the local weather data in conjunction with the actual animal, feed, bedding, ventilation and manure management conditions, Manure-DNDC simulated daily fluxes of NH₃, CH₄, CO₂ and N₂O from the barn. Manure-DNDC estimated NH₃ fluxes mainly from the manure deposited in the barn. The modeled NH₃ production was sensitive to the temperature in the barn. The modeled pattern and magnitudes of NH₃ fluxes are well in agreement with observations (Fig. 7a). The modeled GHGs came from two sources, i.e., the animal metabolic processes (e.g., respiration

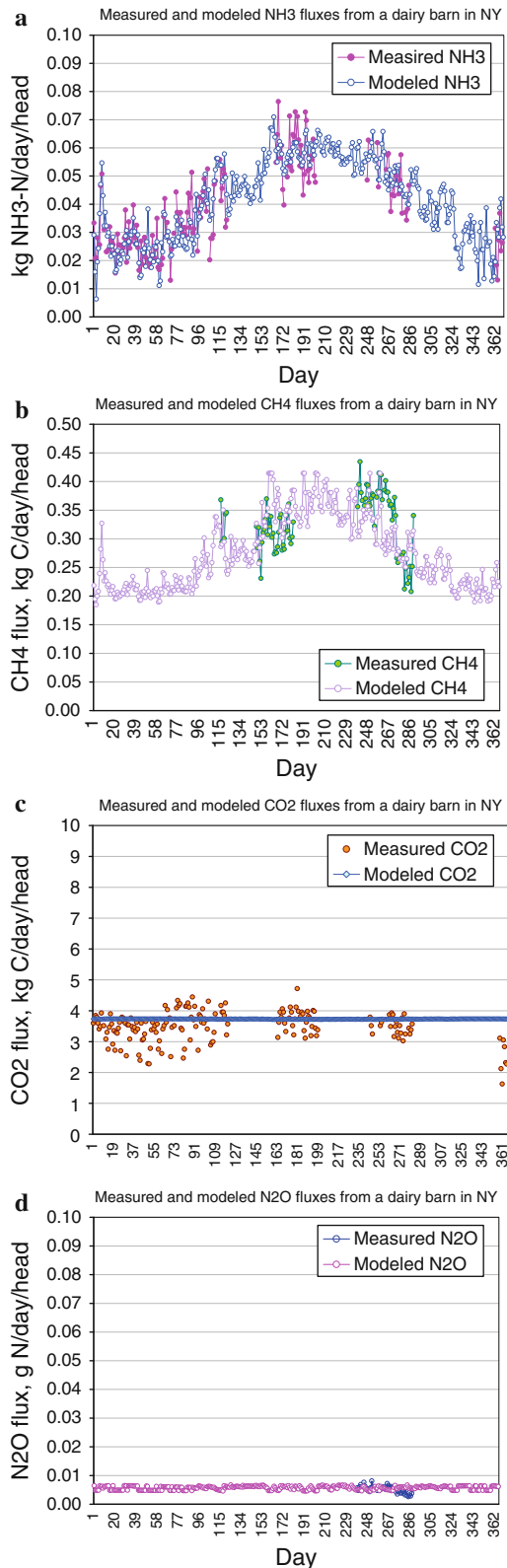


Fig. 7 Observed and modeled NH₃ (a), CH₄ (b), CO₂ (c) and N₂O (d) fluxes from a dairy barn in New York. The modeled pattern and magnitude of NH₃ or CH₄ fluxes are in agreement with observations while the model failed to simulate the variations in observed CO₂ fluxes

and enteric emission) and the manure lying on the floor. Since the feed rate, milk production and meat gain were set constant, the modeled respiration CO₂, enteric CH₄ and enteric N₂O were constant at 3.7 CO₂-C, 0.17 CH₄-C and 0.005 kg N₂O-N/head/day, respectively throughout the year. However, the modeled gas fluxes from the floor varied driven by the biogeochemical reactions occurring in the manure. The measured CH₄ fluxes showed a clear seasonal pattern, which was apparently related to the variation of temperature in the barn.

The measured CH₄ fluxes were in the range of the modeled results (Fig. 7b). The modeled daily CH₄ fluxes consisted of two components including a constant enteric source of 0.17 kg CH₄-C/head/day and a manure source varying between 0 and 0.22 kg CH₄-C/head/day. The modeled CO₂ emissions from the barn were dominated by the animal respiration CO₂ fluxes (about 3.7 kg CO₂-C/head/day). The modeled decomposition-induced CO₂ fluxes were low, accounting for only 1 % of the respiration CO₂, due to the high manure moisture on the floor. The modeled daily CO₂ fluxes didn't show any seasonal pattern due to the constant animal respiration rate. However, the measured CO₂ fluxes varied between 2.2 and 4.5 kg CO₂-C/head/day (Fig. 7c). The observed variation in CO₂ is likely caused by variation in the animal respiration rate, which is a physiological issue beyond capacity of the current version of Manure-DNDC. The model predicted N₂O fluxes, primarily from the enteric source, were relatively low with a constant emission rate which was in agreement with the limited observation data (Fig. 7d).

Case 3 NH₃ emissions from dairy barns in Indiana.

As part of the National Air Emissions Monitoring Study (NAEMS) program, daily NH₃ volatilization fluxes were measured from two freestall barns in Indiana (Site IN5B) during September 12, 2007 to September 12, 2009 (Lim et al. 2010 report). There were 1,600 dairy cows in each of the barns with a feeding rate 9.8–10.9 kg DM/head/day including 12.2 % CP. The housing area was 472 m long × 29 m

wide with a concrete floor. The barn was mechanically ventilated at a rate of 0.2 m³/s. Manure was removed from the freestall barns by scraping. All manure was then fed into a digester that produced methane gas to run three generators that provided electricity for the farm. Solids from the digester effluent were separated, and the liquid was stored in a two-stage lagoon. Manure liquid was either irrigated onto or injected into land in the surrounding area. The separated digested solids were used as bedding in the freestall barns.

Because the two barns shared similar geometry and technical specifications, a virtual barn was set with the averages of the two for simulation. Driven by the local weather data and management conditions, Manure-DNDC calculated daily NH₃ fluxes from the barn. Both the modeled and measured results showed a clear seasonal pattern, which was apparently related to the variations in temperature (Fig. 8). The modeled NH₃ fluxes were in agreement with observations regarding their patterns and magnitudes.

Case 4 NH₃ emissions from dairy barns in Wisconsin.

Under the National Air Emissions Monitoring Study (NAEMS) program, daily NH₃ volatilization fluxes were measured from two freestall barns (B1 and B2) in Wisconsin (Site WI5B) during September 12, 2007 to October 31, 2009 (Cortus et al. 2010). The capacities of B1 and B2 were 275 and 375 cows, respectively. The feeding rate was 11.3 kg DM/head/day with 11.7 % CP. The housing area was 92 m long × 28 m wide for B1 and 107 m long × 30 m wide for B2. The housing floor was concrete. Manure

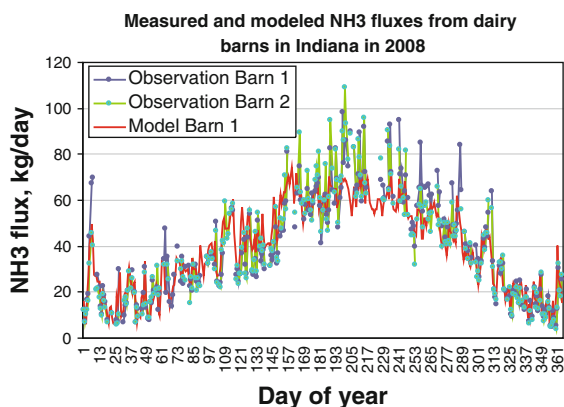


Fig. 8 Comparison between observed and modeled NH₃ fluxes from two dairy barns with capacity of 1,600 cows in Indiana

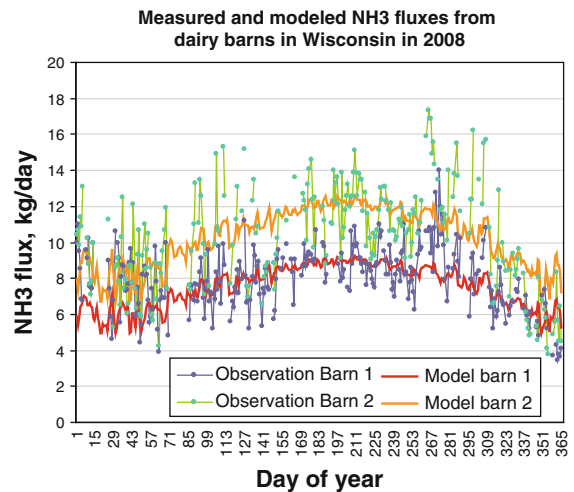


Fig. 9 Comparison between measured and modeled NH₃ fluxes from two dairy barns with herd size of 275 and 375 cows, respectively in Wisconsin in 2008

from the barns was removed by flushing three times per day during the first year and scrape system was used during the second year. The manure flushed from the barns and other feedlot places (e.g., parlor, holding pen) flowed through a solids separator, from which the solids were removed and stacked on a pad until they were spread on fields. The liquid effluent from the solids separator was pumped back into the vertical tanks for reuse to flush the barns. Once a week, enough water was removed from the lagoon and added to the flush tanks to make up for water lost in the recycled flush system. The ventilation rate of Barn 1 ranged from 17 m³s⁻¹ in winter to 355 m³s⁻¹ during the summer. The ventilation rate of Barn 2 ranged from 26 m³s⁻¹ in winter to 378 m³s⁻¹ during the summer.

It is interesting to compare the NH₃ fluxes measured in the Wisconsin farm (WI5B) in this case with that measured at the Indiana farm (IN5B) in Case 3. The barn NH₃ emissions in the two farms differed on not only in their magnitudes but also in the annual pattern. The herd sizes of IN5B and WI5B were 1,600 and 300 cows, respectively that explained the difference in the magnitude of the measured NH₃ fluxes. However, while the NH₃ fluxes substantially decreased during the winter in the Indiana barns, the NH₃ fluxes measured in Wisconsin remained relatively constant (Fig. 9). Manure-DNDC simulated the Wisconsin barn by setting the barn management

conditions following the actual practices including the manure liquid recycling. The modeled data indicated that the recycling of manure liquids for flushing increased its actual residence time in the barns, and its physical disturbance during the flushing operation elevated the volatilization rate of NH_3 from the liquids. These impacts overwhelmed the effect of temperature on NH_3 volatilization from the Wisconsin barns.

Case 5 N_2O , NH_3 and CO_2 emissions from aerobic compost.

A 6-day experiment was conducted to test impacts of rainfall events on N_2O , NH_3 and CO_2 emissions from aerobic compost (Krauter personal communication). The experiment was carried out at the California State University at Fresno in November 2006. A 254 mm artificial rainfall was applied on a 15 cm layer of undisturbed, composted manure in a small exercise corral at a dairy. Fluxes of N_2O , NH_3 and CO_2 were measured before and after the artificial rainfall event at times 0, 1, 2.5, 4, 7, 20, 21, 24, 26 and 93 h after the event. The field data indicated that the rainfall stimulated N_2O and CO_2 emissions (Fig. 10a, b), but depressed NH_3 fluxes for the first 2 days following the rainfall event (Fig. 10c).

The case was simulated with Manure-DNDC by setting the experimental compost at 5,200 kg dry matter (DM) with a density of 200 kg DM/m³. The initial moisture was low (0.2 WFPS). The rainfall was created on the second day of the 6-day experiment. In the simulation, the addition of the 254 mm of water elevated the moisture of the compost, and hence stimulated the decomposers and increased the anaerobic microsites for a higher activity of denitrifiers. On day 1 prior the watering, the modeled CO_2 flux was about 10 g C/m²/day and N_2O about 0.004 g N/m²/day. On the first day and second day post-watering, the modeled CO_2 and N_2O fluxes increased to 110 g C/m²/day and 0.07 g N/m²/day, respectively. For the same time period of the 3 days, NH_3 fluxes decreased from 0.9 to 0.2 g N/m²/day. The modeled data indicated that the decrease in NH_3 flux was due to the dilution of the dissolved NH_4^+ and NH_3 in the manure liquid. The modeled variations and magnitudes of CH_4 , CO_2 and NH_3 were in agreement with observations for the first 3 days of the experiment. During the rest of the experimental period (i.e., from day 4 to day 6), the N_2O fluxes decreased to

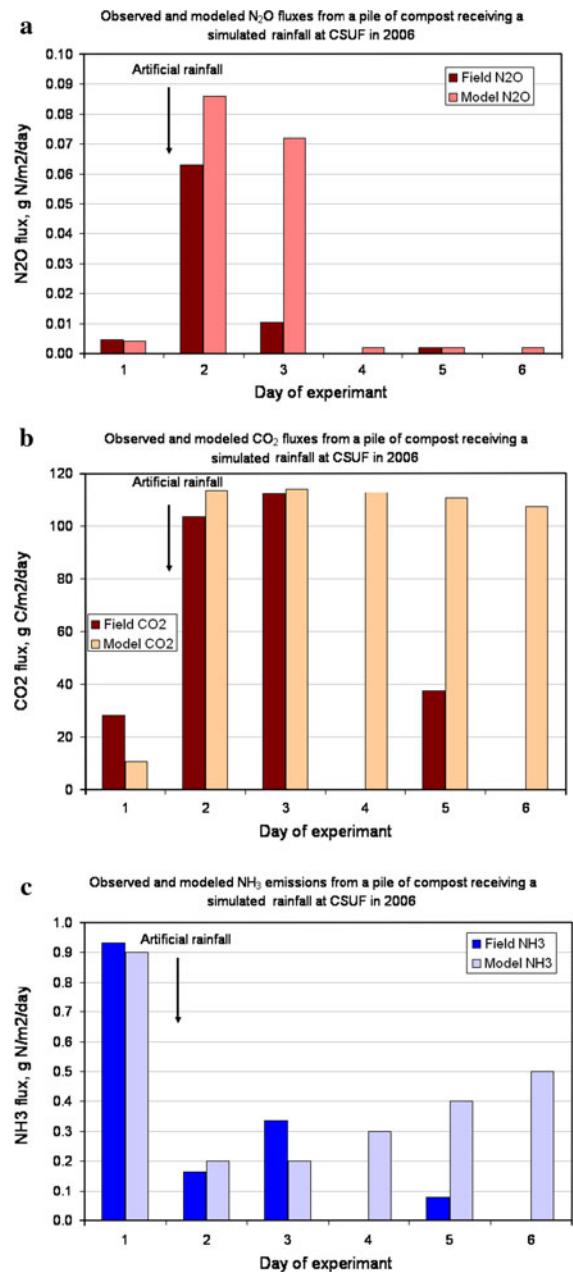
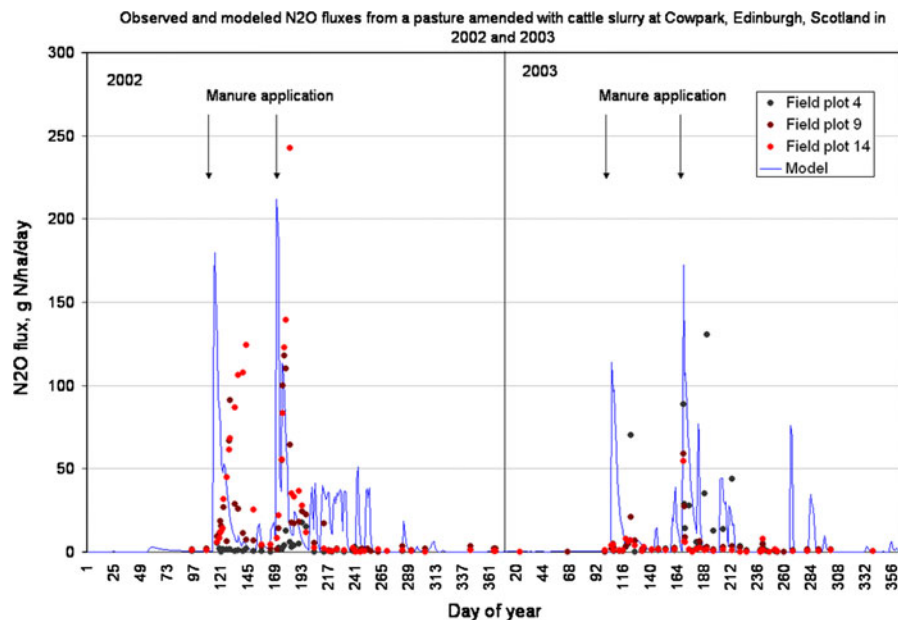


Fig. 10 Comparison between observed and modeled N_2O , CO_2 and NH_3 fluxes from a pile of aerobic compost affected by an artificial rainfall event in California State University at Fresno in 2006

0.002 g N/m²/day for both observation and modeled results; however, the modeled CO_2 emissions remained high and NH_3 fluxes gradually resumed which did not match observations (Fig. 10c). The discrepancy between observation and modeled results

Fig. 11 Manure-DNDC captured the pick emissions of N_2O from a perennial pasture amended with cattle slurry in Cowpark, Edinburgh, Scotland in 2002–2003



could be related to imperfect simulation of the compost moisture dynamics.

Case 6 N_2O emissions from a pasture amended with cattle slurry in Scotland.

Rees and his colleagues measured N_2O emissions from a perennial pasture amended with cattle slurry in Cowpark, Edinburgh, Scotland in 2002–2003 (Bob Rees, personal communication). The slurry applications in the 2 years used the same application rates and dates (2,508 and 2,507 kg C/ha on April 15 and June 18, respectively) but differed in manure constituents. The slurry had a C/N ratio of 9.5 in 2002 but 16.6 in 2003. The observed N_2O fluxes in 2002 were higher than those in 2003.

Manure-DNDC partitions fertilizer manure into soil organic pools based on its C/N ratio. The lower the C/N ratio, the more of the manure allocated into the labile SOC pool. In 2002, the manure contained more N and thus more was allocated into the labile pool which was subject to faster decomposition, and hence led to more N available for nitrification and denitrification. The model simulation basically captured the high emission peaks following the manure applications as well as the difference between 2002 and 2003 (Fig. 11).

Case 7 N fluxes from a swine farm in North Carolina.

A 2-year experiment was conducted on a swine farm in the Coastal Plains of North Carolina in 1997–1998 (Harper et al. 2004). This farm was a 1200 sow farrow-to-finish operation. The waste produced in the barn was directly transported to the lagoon for storage. The pigs were fed 8 kg DM/head/day with 35 % CP. The naturally ventilated barn had a slatted floor with an under-floor gutter for waste collection. No bedding was applied. The feces and urine were collected from both the floor and gutter, mixed and then transferred to the lagoon in a daily time step. The dimension of lagoon was $256 \times 85 \times 3.1$ m with a capacity of 67,456 m^3 and a surface area of 21,760 m^2 . The uncovered lagoon received rain water and was subject to evaporation. About 20 % of the slurry stored in the lagoon was removed to the field every 100 days which gave an average life time of the slurry in the lagoon of 1.5 years. The researchers measured (1) N contents in the feed, milk, meat, feces, urine, lagoon slurry, and field crop and soil, and (2) emissions of NH_3 , N_2O and N_2 from the feedlot, lagoon and field where the lagoon slurry was applied as fertilizer. Based on the 2-year measurements, they closed the N budget within the farm scale. The field data indicated that the feedlot and lagoon shared similar magnitudes of NH_3 emissions and denitrification-induced N_2 dominated N efflux from the lagoon (Harper et al. 2004).

We simulated this case with Manure-DNDC by constructing a virtual swine farm consisting of a barn, a lagoon and a crop field. The modeled barn and lagoon had the same specifications as described by the researchers (Harper et al. 2004). The field (10 ha) produced corn from May 1st to October 1st using natural rainfall. The field soil was a loam with pH 7.0, soil organic carbon (SOC) content of 0.01 kg C/kg, and bulk density of 1.4. The daily weather data of 1998 for Greenville, NC was used to provide air temperature, precipitation and wind speed data for the simulation. A 1 year simulation was conducted, and the model predicted daily C, N and water fluxes for the barn, lagoon and field were recorded for comparison.

Both the observations and modeled results indicated that NH_3 volatilization dominated N losses from the barn and following field application. Manure-DNDC simulated high dinitrogen (N_2) emissions from the lagoon due to denitrification (Fig. 12). The modeled magnitudes of the N fluxes were basically in agreement with observations although discrepancies existed. For example, the modeled N_2 flux from the lagoon was lower than observed by 34 % while the modeled NH_3 flux from lagoon was higher than observed by 28 %. The discrepancy could be related to the modeled chemical composition of the effluent from the housing facility. Manure-DNDC could have underestimated the nitrification rate in the barn and hence led to less nitrate in the effluent slurry transported to the lagoon. Adjusting the feedlot environmental conditions by elevating temperature

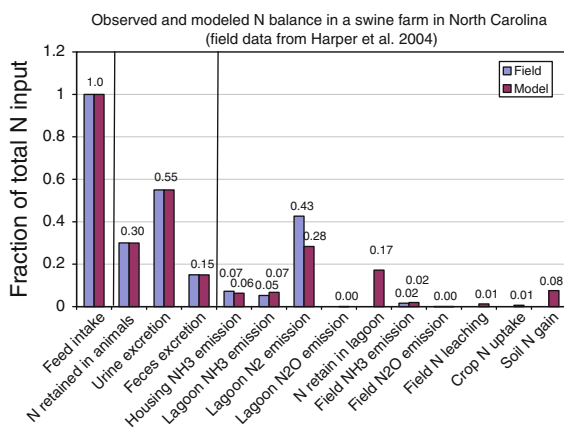


Fig. 12 Comparison between observed and modeled N fluxes for a swine farm in North Carolina. The modeled magnitudes of the N fluxes were basically in agreement with observations although discrepancies existed at the farm scale

or Eh could accelerate nitrification, increase nitrate content in the effluent, and finally enhance the denitrification occurring in the lagoon. In comparison with the measured data, the modeled results provided more information about N fluxes at the farm scale. For example, the modeled data indicated that there was about 15 tons of organic and inorganic N accumulated in the soil and about 2,500 kg of N lost through leaching. This additional information could help provide a more broad assessment of ecosystem services for the swine farm.

Among the seven test cases described above, six focused on the individual farm components of a feedlot or barn (in UC-Davis, New York, Indian and Wisconsin), compost pile (CSU-Fresno) and cropping field (Scotland), and one on multiple components including the barn, lagoon and field (North Carolina). Driven by the local climate, soil and farm management practices, Manure-DNDC simulated CO_2 , CH_4 , N_2O and NH_3 emissions from the farm components without any adjustments to the models internal parameters. The model simulations generally captured the magnitudes and patterns observed across the seven farms. The results imply that the biogeochemical reactions as well as the environmental factors embedded in Manure-DNDC can cover the major processes governing GHG and NH_3 emissions from a range of livestock farms.

It is not surprising to see discrepancies existing between the simulated and measured data. The uncertainty of modeling can come from a number of sources. Most management practices in animal farms are variable in time and space. However, the heterogeneity was ignored in the simulation tests so that the modeled results provided only an average situation for comparison to measured data at specific sites. This issue challenges manure modeling studies. We will need more observations and continuous model improvements to tackle the challenge.

Predicting impacts of management alternatives on farm air emissions

A sensitivity test was conducted by running Manure-DNDC for a hypothetical farm with baseline management practices typical for the dairy farms in the U.S. We assumed the farm was located in northern New York, and consisted of a freestall barn, a lagoon and a

crop field. The barn held 1,100 dairy cows with a feeding rate of 20 kg DM/head/day and CP concentration of 18 % the year around. The barn had a concrete floor with a surface area of 3,850 m². The barn was ventilated with fans. Bedding was applied with 2,500 kg DM of straw (C/N ratio 35) every day. The solid and liquid wastes are mixed and removed to the lagoon daily. The open lagoon had a capacity of 18,535 m³ with a surface area of 300 m². The slurry stored in the lagoon was removed every 120 days and applied to the surface of the crop fields (485 ha). The crop fields were planted in corn (243 ha) and soybean (242 ha) with conventional tillage. The portions of the slurry manure applied on the corn and soybean plots were 80 and 20 %, respectively. 90 % of the above-ground biomass of corn was harvested and used as feed within the farm scale. All of the soybean grain was harvested and fed on the farm. The field soil was a sandy clay loam with a pH of 6.5, bulk density of 1.4, and organic C content of 0.015 kg C/kg. Daily weather data of 2008 collected from the climatic station at Onondaga, NY was used to drive the simulation. Manure-DNDC was run with the baseline input data to produce daily and annual C and N fluxes for each of the farm components. The farm-scale fluxes were calculated by summing up the fluxes from the components. The modeled GHG and NH₃ fluxes from the farm are summarized in Table 6 and reported on an annual basis as follows:

1. The 1,100 dairy cows consumed 3,212 tons C (equivalent to 8,030 tons DM) and 231 tons N (equivalent to 1,444 tons CP) in feed, which produced milk (containing 231 tons C and 58 tons N), meat (42 tons C and 12 tons N), urine (101 tons C and 81 tons N), feces (1,294 tons C and 81 tons N), animal respiration (1,358 tons C), enteric CH₄ (186 tons C) and enteric N₂O (0.1 tons N);
2. The farm received 365 tons C and 10 tons N through purchased bedding;
3. The farm-scale CO₂ emission was 246 tons C including 1358, 18, 0.09, –1310 and 180 tons C from animal respiration, barn manure decomposition, lagoon, corn field and soybean field sources, respectively;
4. The farm-scale CH₄ emission was 196 tons C including 186, 10 and –0.3 tons C from enteric, lagoon and crop field sources, respectively;

5. The farm-scale N₂O emission was 7 tons N including 6, 0.03 and 0.8 tons N from the barn, lagoon and crop field sources, respectively;
6. The farm-scale NH₃ emission was 77 tons N including 23, 40 and 14 tons N from the barn, lagoon and crop field sources, respectively;
7. About 3 tons N was lost through leaching from the crop fields;
8. The field soils gained 1,130 tons C as a balance between the soil C inputs from manure application (1,705 tons C) and crop residue incorporation (705 tons C) and the soil C outputs through soil heterotrophic respiration (1,280 tons C);
9. The field soils gained 54 tons N as a balance between the soil N inputs from manure application (98 tons N), atmospheric deposition (4 tons N), crop N fixation (2 tons N) and crop residue incorporation (12 tons N) and the soil N outputs through crop uptake (44 tons N), N gas emission (17 tons C) and N leaching loss (3 tons N);
10. The harvested crop biomass contained 2,160 tons C (equivalent to 5,400 tons DM) and 46 tons N (equivalent to 288 tons CP). When all the harvested biomass was utilized as livestock feed on the farm, there was a deficit of 1,052 tons C and 185 tons N for feed. The farmer had to purchase 2,630 tons DM and 1,158 tons CP of feed from outside sources to meet the gap.

In summary, the farm annually emitted 246 tons CO₂–C, 196 tons CH₄–C and 7 tons N₂O–N, which were 901, 6531 and 3434 tons CO₂-equivalent (CO₂e) using IPCC method Global Warming Potential factors (i.e., 100-year horizon criteria: 1 kg CH₄ or N₂O equivalent to 21 or 310 kg CO₂e, respectively; IPCC 1996a). The farm as a whole contributed 10,866 CO₂e with 60 % from CH₄ emission, 32 % from N₂O and 8 % from CO₂. The farm NH₃ emissions mainly came from the lagoon (52 %) followed by the barn (30 %) and crop fields (18 %). About 3 tons N was lost through nitrate leaching from the farm, which could contaminate the adjacent surface water or groundwater.

There are technical potentials to mitigate GHG and NH₃ emissions from animal farms. Some of the measures are related to animal physiology including breeding and utilization of ionophores, antibiotics, vaccine, tannins etc. to change the rumen microbe population/metabolisms; and some are related to farm

Table 6 Manure-DNDC modeled annual C and N fluxes for a dairy farm with baseline and alternative management scenarios

Scenario	BASE		AL-1		AL-2		AL-3		AL-4	
	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)
<i>Feed input</i>										
Feed	3212000	231263	3212000	192720	3212000	231263	3212000	231263	3212000	192720
Bedding	365000	10429	365000	10429	365000	10429	365000	10429	365000	10429
Sum	3577000	241692	3577000	203149	3577000	241692	3577000	241692	3577000	203149
<i>Production</i>										
Milk	231263	57816	192720	48180	231263	57816	231263	57816	192720	48180
Meat	42048	11563	35040	9636	42048	11563	42048	11563	35040	9636
Sum	273311	69379	227760	57816	273311	69379	273311	69379	227760	57816
<i>Excreta</i>										
Urine	101106	80885	84255	67404	101106	80885	101106	80885	84255	67404
Feces	1294153	80885	1356564	67404	1294153	80885	1294153	80885	1356564	67404
Sum	1395259	161770	1440819	134808	1395259	161770	1395259	161770	1440819	134808
<i>CO₂ flux</i>										
Respiration	1357511		1388499		1357511		1357511		1388499	
Feedlot floor	18415		14272		18415		18415		14272	
Lagoon	94		73		89		94		74	
Corn field	(1310307)		(1331754)		(1247995)					
Soybean field	180101		173746		194787					
Alfalfa field							(1556910)		(1740847)	
Sum	245814		244836		322807		(180890)		(338002)	
<i>CH₄ flux</i>										
Enteric	185920		154933		185920		185920		154933	
Feedlot floor	0		0		0		0		0	
Lagoon	10323		8664		21319		10323		18966	
Corn field	-155		-155		-156					
Soybean field	-157		-157		-157				(306)	
Alfalfa field							(306)			
Sum	195931		163285		206926		195937		173593	
<i>N₂O flux</i>										
Enteric N ₂ O		116		96		116		116		96

Table 6 continued

Scenario	BASE		AL-1		AL-2		AL-3		AL-4	
	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)	C (kg C/year)	N (kg N/year)
Feedlot floor	6397	5826	6397	5826	6397	5826	6397	5826	6397	5826
Lagoon	31	16	31	16	31	16	31	16	31	16
Corn field	397	343	397	343	466	0	0	0	0	0
Soybean field	392	382	392	382	415	0	0	0	0	0
Alfalfa field										
Sum	7333	6663	7425	6663	7425	6630	7230	6630	7230	6630
<i>NH₃ flux</i>										
Feedlot floor	22574	18454	22574	18454	22574	18454	22574	18454	22574	18454
Lagoon	39926	32736	39926	32736	16867	39926	16867	39926	16867	39926
Corn field	11769	9684	11769	9684	16637	15950	16637	15950	16637	15950
Soybean field	2938	2598	2938	2598	4295		4295		4295	
Alfalfa field										
Sum	77207	63472	60373	63472	60373	15207	77253	15207	77253	49611
<i>N leaching loss</i>										
Corn field	1136	1046	1136	1046	1328	0	0	0	0	0
Soybean field	2309	2240	2309	2240	2404	0	0	0	0	0
Alfalfa field										
Sum	3445	3286	3732	3286	3732	1961	1910	1961	1910	1961
<i>Forage production</i>										
Corn field	1905637	20919	1909074	20919	1912084	20952	1800558	72267	183682	72256
Soybean field	254305	25430	254311	25431	254305	25431	1800558	72267	183682	72256
Alfalfa field							1800558	72267	183682	72256
Sum	2159942	46311	2163385	46350	2166389	46383	1800558	72267	183682	72256

Table 7 Manure-DNDC modeled annual GHG fluxes from a dairy farm with baseline and alternative management scenarios

	BASE		AL-1		AL-2		AL-3		AL-4	
	Flux	CO ₂ e	Flux	CO ₂ e	Flux	CO ₂ e	Flux	CO ₂ e	Flux	CO ₂ e
CO ₂ , ton C	246	901	245	898	323	1184	−181	−663	−338	−1239
CH ₄ , ton C	196	6531	163	5443	207	6898	196	6531	174	5786
N ₂ O, ton N	7	3434	7	3120	7	3477	7	3386	7	3105
Net GHG, ton CO ₂ e		10866		9461		11558		9254		7652

management alternatives from feed composition to manure application method. As a biogeochemical model, the current version of Manure-DNDC only focuses on the later. Three management alternatives were designed to test their impacts on GHG and NH₃ emissions at the farm scale. The first alternative (AL-1) was to reduce the feed CP concentration from the baseline 18 to 15 %; the second alternative (AL-2) was to cover the lagoon to reduce NH₃ volatilization; the third option (AL-3) was to plant higher-yielding alfalfa (20 tons DM/ha) in the field to create more DM and CP for feed; and the fourth option (AL-4) was designed by combining the alternative practices applied in AL-1, AL-2 and AL-3. Manure-DNDC was used to simulate each of the four alternative scenarios for 1 year. The annual fluxes of C and N predicted by Manure-DNDC with the baseline and alternative scenarios for the farm were recorded in Table 6 for comparison.

Scenario AL-1 represented an upstream alternative management practice with a change in feed quality. The reduction in the feed CP concentration from 18 to 15 % reduced the total annual feed N input by 39 tons N. This option reduced the urine and feces N content by 27 tons N from 162 to 135 tons N per year, and this affected the N gas fluxes from all farm components. For example, NH₃ volatilization fluxes decreased by 18 % for all the facilities; and N₂O emissions from the enteric source, barn, lagoon and crop field decreased by 17, 9, 48 and 18 %, respectively. However, the modeled results indicated a decrease in milk production due to the degradation in the feed quality although it may not occur in the actual farmers' practice. Since the crop fields received excess manure N already with the baseline scenario, AL-1 didn't affect the crop yields (Table 6).

Scenario AL-2 added a cover to the lagoon which reduced the lagoon NH₃ flux by 58 % but doubled the lagoon CH₄ flux due to the increased anaerobic conditions. Since more N was removed from the

lagoon to the crop fields, the field NH₃ flux increased by 43 % and the soil N leaching flux increased by 8 % (Table 6).

In scenario AL-3, the 485 ha of crop field was planted with alfalfa, which required more N from both the soil and the atmosphere and produced more root biomass to increase soil C sequestration. This option significantly increased the soil C sequestration rate by 48 %, reduced the soil N leaching loss by 45 %, and increased the CP content in the forage produced from the field by 56 % (Table 6).

AL-4 was set by combining the alternative practices applied in AL-1, AL-2 and AL-3. As expected, AL-4 affected all C and N fluxes across the farm components. With this scenario, the farm was converted from a source to a sink of atmospheric CO₂; CH₄ emissions decreased from 196 to 174 tons C; N₂O emission decreased from 7.3 to 6.6 tons N; NH₃ emission decreased from 77 to 50 tons N; and soil N leaching loss decreased from 3.4 to 2.0 tons N (Table 6).

By converting the modeled CO₂, CH₄ and N₂O fluxes into CO₂ equivalent, we concluded that the farm as a whole emitted 10,866, 9,461, 11,558, 9,254 and 7,652 tons CO₂e per year under the baseline, AL-1, AL-2, AL-3 and AL-4 management scenarios, respectively. The NH₃ fluxes emitted from the farm were 77, 63, 60, 77 and 50 tons N per year under the baseline, AL-1, AL-2, AL-3 and AL-4 management scenarios, respectively. The multi-change scenario AL-4 could reduce GHG emissions by 30 % and NH₃ by 36 % at the farm scale (Table 7).

Discussions

Contemporary agriculture finds itself in the dilemma of nutrient management. On one hand a great amount of synthetic fertilizer is required to support the food or forage production in the cropping systems. On the other

hand a lot of manure nutrients are handled as waste in the livestock operation systems, which has the potential to pollute the environment. The nutrient management between livestock and cropping systems needs to be balanced to reduce their environmental impact. However, efforts of this type have been hampered due to the lack of tools that predict impacts of not only the single management practices but also the coherence between livestock and cropping ecosystems on both production and environmental safety. Manure-DNDC is a product resulting from our long-term efforts on modeling terrestrial ecosystems based on classical knowledge of sciences. Manure-DNDC was developed as a biogeochemical model with a focus on the biochemical and geochemical processes that govern the transport and transformation of C, N, P and water in the manure life cycle. Built upon the principles of thermodynamics and chemical reaction kinetics, the model can be applied to various environmental conditions across livestock facilities as well as cultivated soils. This capacity enables the model to quantitatively link nutrient cycling between the two major agricultural ecosystems at farm or regional scales.

Air emission from livestock farms is a complex phenomenon, which involves multiple processes driven by multiple environmental factors varying differently across the farm component facilities. The sensitivity test described in the present paper demonstrates how a model tool such as Manure-DNDC can handle the complexity. The case study evaluation shows that change in a specific management practice can simultaneously affect a number of C or N fluxes released from several components of the livestock system. By modeling GHG emissions, NH_3 volatilization, nitrate leaching, and even crop yield in parallel, Manure-DNDC provides a wide spectrum of data to help assess the best management practices based on their impacts

on a relatively complete span of ecosystem services. Of course, when the model is used for this purpose, the candidate scenarios of alternative management practices need to be carefully designed based on not only theoretical analysis but also field realities.

However, the Manure-DNDC model reported in this paper is in its early stage of development. There are some necessary features missing in the initial version. For example, the current version lacks nutritional functions for livestock, which should play a crucial role in defining the nutrients and quantity of excreta by linking feed to animal metabolisms and animal performance, a key to sustainability. In addition, energy use is not included in the model so that indirect GHG emissions induced by transportation, machinery, fertilizer production, feed import etc. cannot be calculated. Finally, an economic analysis is not included yet. There could be more features beyond our current considerations, which need to be included in the model. However, by publishing this paper with the model, we expect comments and suggestions from the users for further development. As public domain software, the Manure-DNDC model with a User's Guide is available at <http://www.dndc.sr.unh.edu>.

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Appendix 1

See Table 8.

Table 8 Equations of biogeochemical processes parameterized in Manure-DNDC

Description	Equation
1. Partitioning of feces to litter and humads pools	$\text{HumadsN} = (\text{rcnrr} \times \text{FecesN} - \text{FecesC})/(\text{rcnrr} - \text{rcnh});$ $\text{LitterN} = \text{FecesN} - \text{HumadsN};$ $\text{LitterC} = \text{rcnrr} \times \text{LitterN};$ $\text{HumadsC} = \text{rcnh} \times \text{HumadsN};$
	where FecesC, feces C content; FecesN, feces N content; rcnrr, resistant litter C/N ratio; rcnh, humads C/N ratio; HumadsC, humads C content; HumadsN, humads N content; LitterC, litter C content; LitterN, litter N content

Table 8 continued

Description	Equation
2. Decomposition rate of manure organic carbon pool	$dC/dt = CNR \cdot \mu \cdot (S \cdot k_1 + (1 - S) \cdot k_r) \cdot C$ <p>where C, decomposed manure organic C (kg C/kg manure per day); t, time (day); S, labile fraction of organic C compounds in the pool; (1 - S), resistant fraction of organic C compounds; k₁, specific decomposition rate (SDR) of labile fraction (1/day); k_r, SDR of the resistant fraction (1/day); μ, temperature and moisture reduction factor; CNR = 0.2 + 7.2/(CP/NP), C:N ratio reduction factor; CP, C produced by potential residue decomposition per day (without CNR reduction factor) (kg C/ha); NP, N produced by potential residue decomposition per day plus free NH₄⁺ and NO₃⁻ in soil (kg N/ha). C/N ratio = 02.35, 20, 20, 8, 8, 8 and 8; SDR = 0.074, 0.074, 0.02, 0.33, 0.04, 0.16 and 0.006 (1/day) for very labile litter, labile litter, resistant litter, labile microbes, resistant microbes, labile humads and resistant humads, respectively</p>
3. Urease activity	$UREASE = k1 \times DOC \times WFPS \times T,$ <p>where UREASE is urease activity (percent of urea hydrolyzed per day), DOC is dissolved organic carbon content (kg N/ha), WFPS is water-filled porosity, T is temperature (°C), and k1 is a coefficient (0.9 ha/kg/°C)</p>
4. Hydrolysis rate of urea	$dUrea = [Urea] \times UREASE,$ <p>where dUrea is daily hydrolyzed urea which is totally converted into NH₄⁺, and [Urea] is concentration of urea (kg N/ha)</p>
5. NH ₄ ⁺ /NH ₃ equilibrium	$NH_4^+ = NH_3 + H^+;$ $K_a = [NH_4^+][OH^-]/[NH_3(l)],$ $[H^+] = 10^{-pH},$ $H_2O = H^+ + OH^-;$ $K_w = [H^+][OH^-],$ $K_a = (1.416 + 0.01357 \times T) \times 10^{-5},$ $K_w = 10^{(0.08946 + 0.03605 \times T)} \times 10^{-15}$ <p>where K_a is equilibrium constant, K_w is water dissociation constant, [NH₄⁺], [OH⁻] and [NH₃(l)] are NH₄⁺, OH⁻ and NH₃(l) concentrations (mol/l) in manure water, pH is manure pH, T is manure temperature</p>
6a. NH ₃ diffusion from the bulk liquid to the interface liquid phase in manure liquids	$F_l = K_l \times ([NH_3]_{bl} - [NH_3]_{il}),$ <p>where F_l, NH₃ diffusion rate in liquid phase (kg N/m²/h); K_l, NH₃ mass transfer coefficient in the liquid boundary layer; [NH₃]_{bl}, NH₃ concentration in the bulk liquid phase (kg N/m³); [NH₃]_{il}, NH₃ concentration in the interface liquid phase (kg N/m³)</p>
6b. NH ₃ transfer from the interface liquid phase to the bulk air	$F_g = K_g \times ([NH_3]_{ig} - [NH_3]_{ag}),$ <p>where F_g, NH₃ transfer rate from the interface liquid phase to the bulk air (kg N/m²/h); K_g, NH₃ mass transfer coefficient in the air boundary layer; [NH₃]_{ig}, NH₃ concentration in the interface gas phase (kg N/m³); [NH₃]_{ag}, NH₃ concentration in the air (kg N/m³)</p>
6c. Equilibrium between NH ₃ in the interface liquid and NH ₃ in the interface gas phase	$[NH_3]_{ig} = K_h \times [NH_3]_{il},$ <p>where [NH₃]_{ig}, NH₃ concentration in the interface gas phase (kg N/m³); [NH₃]_{il}, NH₃ concentration in the interface liquid phase (kg N/m³); K_h, Henry's coefficient</p>

Table 8 continued

Description	Equation
7. Nitrification	$\text{GROWTHn} = 0.0166 \times (\text{DOC}/(1 + \text{DOC}) + \text{Ft}/(1 + \text{Ft}));$ $\text{DEATHn} = 0.008 \times \text{nitrifier} \times 1/(1 + \text{DOC})/(1 + \text{Ft});$ $\text{dNNO} = K_{35} \cdot \text{NH}_4(t) \cdot \text{nitrifier} \cdot R_t \cdot R_m;$ <p>where GROWTHn, daily nitrifier growth rate; DEATHn, daily nitrifier death rate; DOC, dissolved organic carbon concentration (kg C/ha); Ft, temperature factor; Nitrifier, nitrifier population (kg C/ha); dNNO, NH_4^+ converted to NO_3^- during time dt (kg N/ha/day); $\text{NH}_4(t)$, available NH_4^+ at time t (kg N/ha); K_{35}, nitrification rate (25 mg/kg manure/day) at 35 °C; R_m, moisture reduction factor; R_t, temperature reduction factors</p>
8a. Denitrifier growth rate:	$(\text{dB}/\text{dt})_g = u_{\text{DN}} \cdot \text{B}(t),$ <p>where $(\text{dB}/\text{dt})_g$, potential growth rate of denitrifier biomass (kg C/ha/day); B(t), total biomass of the denitrifier at time t (kg C/ha); u_{DN}, relative growth rate of the denitrifiers,</p> $u_{\text{DN}} = \text{TE} \cdot (u_{\text{NO}_3} \cdot \text{PH}_{\text{NO}_3} + u_{\text{NO}_2} \cdot \text{PH}_{\text{NO}_2} + u_{\text{N}_2\text{O}} \cdot \text{PH}_{\text{N}_2\text{O}}),$ $u_{\text{N}_x\text{O}_y} = u_{\text{N}_x\text{O}_y, \text{max}} \cdot (C/(K_{c,1/2} + C)) \cdot (\text{N}_x\text{O}_y/(K_{\text{N}_x\text{O}_y,1/2} + \text{N}_x\text{O}_y));$ <p>where $u_{\text{N}_x\text{O}_y}$, rel. growth rate of NO_3^-, NO_2^-, or N_2O denitrifiers; $u_{\text{N}_x\text{O}_y, \text{max}}$, max. growth rate of NO_3^-, NO_2^-, or N_2O denitrifiers; C, concentration of soluble carbon in soil water (kg C/ha); N_xO_y, concentration of NO_3^-, NO_2^-, or N_2O in soil water (kg N/ha); $K_{c,1/2}$, half-saturation value of soluble C in the Monod model (kg C/m³ soil water); $K_{\text{N}_x\text{O}_y,1/2}$, half-saturation value of NO_3^-, NO_2^-, or N_2O in the Monod model (kg N/m³ soil water)</p> $\text{TE} = 2^{(T - 22.5)/10}, \text{ for } T < 60,$ $\text{TE} = 0.0, \text{ for } T \geq 60$ $\text{PH}_{\text{NO}_3} = 7.14 \cdot (\text{PH} - 3.8)/22.8$ $\text{PH}_{\text{NO}_2} = 1.0$ $\text{PH}_{\text{N}_2\text{O}} = 7.22 \cdot (\text{PH} - 4.4)/18.8$ <p>T, soil temperature (°C); PH, soil pH</p>
8b. Denitrifier death rate	$(\text{dB}/\text{dt})_d = M_c \cdot Y_c \cdot \text{B}(t),$ <p>where $(\text{dB}/\text{dt})_d$, death rate of denitrifier biomass (kg C/ha/hr); M_c, maintenance coefficient of carbon (kg C/kg C/h); Y_c, maximum growth yield on soluble carbon (kg C/kg C); B(t), denitrifier biomass at time t (kg C/ha)</p>
8c. Consumption of DOC by denitrifiers	$\text{dC}_{\text{con}}/\text{dt} = (u_{\text{DN}}/Y_c + M_c) \cdot \text{B}(t),$ <p>where C_{con}, consumed soluble C (kg C/ha); u_{DN}, relative denitrifier growth rate; Y_c, maximum growth yield on soluble carbon (kg C/kg C); M_c, maintenance coefficient of carbon (kg C/kg C/h)</p>
8d. Nitrate, nitrite and nitrous oxide consumption:	$\text{d}(\text{N}_x\text{O}_y)/\text{dt} = (u_{\text{N}_x\text{O}_y}/Y_{\text{N}_x\text{O}_y} + M_{\text{N}_x\text{O}_y} \cdot \text{N}_x\text{O}_y/\text{N}) \cdot \text{B}(t) \cdot \text{PH}_{\text{N}_x\text{O}_y} \cdot \text{TE},$ <p>where $Y_{\text{N}_x\text{O}_y}$, maximum growth yield on NO_3^-, NO_2^-, or N_2O (kg C/kg N); N, total nitrogen as NO_3^-, NO_2^-, and N_2O (kg N/ha); $M_{\text{N}_x\text{O}_y}$, maintenance coefficient of NO_3^-, NO_2^-, or N_2O (kg N/kg/h); B(t), denitrifier biomass at time t (kg C/ha); PH, soil pH factor; TE, soil temperature factor</p>
8e. The nitrogen assimilation rate by denitrifiers	$(\text{dN}/\text{dt})_{\text{asm}} = (\text{dB}/\text{dt})_g \cdot (1/\text{CNR}_{\text{DN}}),$ <p>where $(\text{dN}/\text{dt})_{\text{asm}}$, nitrogen assimilation rate by denitrifiers (kg N/ha/day); CNR_{DN}, C/N ratio in denitrifiers (3.45)</p>

Table 8 continued

Description	Equation
9a. Methane production	$\text{CH}_4\text{p} = (1.5 \times \text{DOC} + 0.9 \times \text{CO}_2\text{MAI} = \text{T} \times \text{EXP}((\text{T} - 30)/50)/30 + 0.1, \text{T} \leq 30;$ $\text{MAI} = 30 \times \text{EXP}((30 - \text{T})/50)/\text{T} + 0.1, \text{T} > 30;$ $\text{PHI} = (7/\text{PH}^2 \times \text{EXP}(\text{PH} - 7)), \text{PH} \leq 7;$ $\text{PHI} = \text{EXP}(0.7 \times (7 - \text{PH})), \text{PH} > 7;$ $\text{Ehf} = -0.0042 \times (\text{Eh}/100)^4 + 0.0706 \times (\text{Eh}/100)^3 - 1.557 \times (\text{Eh}/100)^2 - 2.3617 \times (\text{Eh}/100) + 10.359;$ $\text{Eftt} = [(1 - \text{EXP}(-2/\text{NO}_3)) \times 1.5] \times (\text{EXP}(\text{NH}_4/1000))$ <p>where CH_4p is CH_4 production rate (kg $\text{CH}_4\text{-C}/\text{ha}/\text{day}$), Eh manure redox potential (mV), [DOC] concentration of DOC (kg C/ha), $[\text{CO}_2]$ concentration of CO_2 (kg C/ha), MAI microbial activity index, T manure temperature (degree C), PH manure pH</p>
9b. Methane oxidation	$\text{CH}_4\text{o} = .6 \times [\text{CH}_4] \times (.1 + \text{T}/30)^2/\text{EXP}(-(\text{Eh} + 150)/150)$ <p>where CH_4o is CH_4 oxidation rate (kg $\text{CH}_4\text{-C}/\text{ha}/\text{day}$), $[\text{CH}_4]$ is CH_4 concentration (kg $\text{CH}_4\text{-C}/\text{ha}$), and Eh is manure Eh (mv)</p>
9c. Methane diffusion rate	$\text{DIFF}(\text{L}) = (\text{CH}_4(\text{L}) - \text{CH}_4(\text{L} + 1)) \times \text{T},$ <p>where $\text{DIFF}(\text{L})$ is CH_4 flux (kg $\text{CH}_4\text{-C}/\text{day}$) from manure, $[\text{CH}_4(\text{L})]$ and $[\text{CH}_4(\text{L} + 1)]$ are CH_4 concentrations (kg $\text{CH}_4\text{-C}/\text{ha}$) in and outside manure, respectively, T is temperature (degree C), PORO is air-filled porosity</p>

Appendix 2

See Table 9.

Table 9 Feed materials incorporated in Manure-DNDC for calculating feed rates and nutrient contents

	Dry matter (%)	Crude protein (%)	Phosphorus (%)	Sulfur (%)
ALFALFA	90.3	19.2	0.28	0.26
ALMOND	86.9	6.5	0.13	0.04
APPLE	35.9	7.7	0.14	0.07
BAKERY_BYPRODUCT	84.7	12.5	0.36	0.14
BARLEY_GRAIN	91	12.4	0.39	0.12
BARLEY_SPROUTS	90.5	20.1	0.51	0.29
BARLEY_SILAGE	35.5	12	0.3	0.17
BEET_SUGAR	88.3	10	0.09	0.3
BERMUDAGRASS	87.1	10.4	0.27	0.48
BLOOD	90.2	95.5	0.3	0.77
BREWERS_GRAINS	90.7	29.2	0.67	0.38
CANOLA	89.9	20.5	0.68	0.42
CHOCOLATE	95.2	11.9	0.3	0.11
CITRUS	85.8	6.9	0.12	0.1
CORN,_YELLOW_COBS	90.8	3	0.06	0.07
CORN,_YELLOW_DistillersGrains	90.2	29.7	0.83	0.44
CORN,_YELLOW_GlutenFeed	89.4	23.8	1	0.44
CORN,_YELLOW_GlutenMeal	86.4	65	0.6	0.86

Table 9 continued

	Dry matter (%)	Crude protein (%)	Phosphorus (%)	Sulfur (%)
CORN,_YELLOW_GrainCracked	88.1	9.4	0.3	0.1
CORN,_YELLOW_GrainGround	88.1	9.4	0.3	0.1
CORN,_YELLOW_GrainSteam-flaked	88.1	9.4	0.3	0.1
CORN,_YELLOW_GrainRolled	71.8	9.2	0.3	0.1
CORN,_YELLOW_GrainGround	71.8	9.2	0.3	0.1
CORN,_YELLOW_GrainCob	89.2	8.6	0.28	0.09
CORN,_YELLOW_Hominy	88.5	11.9	0.65	0.12
CORN,_YELLOW_SilageImmature	23.5	9.7	0.24	0.14
CORN,_YELLOW_SilageNormal	35.1	8.8	0.26	0.14
CORN,_YELLOW_SilageMature	44.2	8.5	0.25	0.1
COTTON_SEED_WHOLE	90.1	23.5	0.6	0.23
COTTON_SEED_Hulls	89	6.2	0.12	0.07
COTTON_SEED_Meal	90.5	44.9	1.15	0.4
FATS_AND_OILS_CalciumSoaps	95.3	0	0	0
FATS_AND_OILS_Hydrolyzed_tallow_fatty_acids	99.8	0	0	0
FATS_AND_OILS_Partially_hydrogenated_tallow	100	0	0	0
FATS_AND_OILS_Tallow	99.8	0	0	0
FATS_AND_OILS_VegetableOil	100	0	0	0
FEATHERS_Hydrolyzed_meal	93.3	92	0.5	1.39
FEATHERS_Hydrolyzed_meal viscera	91.5	85	0.77	1.75
FISH_BYPRODUCTS_Anchovy_meal	92	71.2	2.69	0.78
FISH_BYPRODUCTS_Menhaden	91.2	68.5	3.05	1.16
GRASSES_COOL_EASON_PastureIntensively Managed	20.1	26.5	0.44	0.2
GRASSES_COOL_EASON_Hay	88.1	10.6	0.23	0.21
GRASSES_COOL_EASON_Hay_immature	84	18	0.34	0.24
GRASSES_COOL_EASON_Hay_mid_maturity	83.8	13.3	0.29	0.24
GRASSES_COOL_EASON_Hay_mature	84.4	10.8	0.26	0.17
GRASSES_COOL_EASON_Silage	36.5	12.8	0.29	0.21
GRASSES_COOL_EASON_Silage_immature	36.2	16.8	0.36	0.21
GRASSES_COOL_EASON_Silage_mid_maturity	42	16.8	0.36	0.21
GRASSES_COOL_EASON_Silage_mature	38.7	12.7	0.31	0.2
GRASS-LEGUME_MIXTURES_Predominantly Grass_Hay_immature	84.3	18.4	0.31	0.28
GRASS-LEGUME_MIXTURES_Predominantly Grass_Hay_mid_maturity	87.3	17.4	0.36	0.27
GRASS-LEGUME_MIXTURES_Predominantly Grass_Hay_mature	84.7	13.3	0.27	0.29
GRASS-LEGUME_MIXTURES_Predominantly Grass_Silage_immature	47.1	18	0.34	0.27
GRASS-LEGUME_MIXTURES_Predominantly Grass_Silage_mid_maturity	44.5	17.6	0.36	0.25
GRASS-LEGUME_MIXTURES_Predominantly Grass_Silage_mature	38.5	15.4	0.33	0.34

Table 9 continued

	Dry matter (%)	Crude protein (%)	Phosphorus (%)	Sulfur (%)
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_Hay_immature	83.1	19.7	0.31	0.27
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_Hay_mid_maturity	85.3	18.4	0.32	0.24
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_HayMature	89.7	18.2	0.37	0.28
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_SilageImmature	45.9	20.3	0.35	0.16
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_SilageMidMaturity	44.1	19.1	0.35	0.26
GRASS-LEGUME_MIXTURES_Mixed Grass_and_Legume_SilageMature	42.8	17.4	0.33	0.31
GRASS-LEGUME_MIXTURES_ Predominantly_Legume_HayImmature	83.8	20.5	0.3	0.2
GRASS-LEGUME_MIXTURES_Predominantly_ Legume_HayMidMaturity	84.2	19.1	0.3	0.26
GRASS-LEGUME_MIXTURES_Predominantly_ Legume_HayMature	84.3	17.2	0.28	0.26
GRASS-LEGUME_MIXTURES_Predominantly_ Legume_SilageImmature	43.2	20	0.36	0.32
GRASS-LEGUME_MIXTURES_Predominantly_ Legume_SilageMidMaturity	43.3	19	0.34	0.25
GRASS-LEGUME_MIXTURES_Predominantly_ Legume_SilageMature	42.9	18.3	0.33	0.26
LEGUMES_FORAGE_PastureIntensivelyManaged	21.4	26.5	0.37	0.31
LEGUMES_FORAGE_Hay_all	87.8	20.2	0.26	0.25
LEGUMES_FORAGE_HayImmature	84.2	22.8	0.31	0.33
LEGUMES_FORAGE_HayMidMaturity	83.9	20.8	0.3	0.31
LEGUMES_FORAGE_HayMature	83.8	17.8	0.28	0.23
LEGUMES_FORAGE_Silage_all	39.1	20	0.32	0.24
LEGUMES_FORAGE_SilageImmature	41.2	23.2	0.36	0.3
LEGUMES_FORAGE_SilageMidMaturity	42.9	21.9	0.35	0.28
LEGUMES_FORAGE_SilageMature	42.6	20.3	0.33	0.28
LINSEED(Flax)	90.3	32.6	0.83	0.37
MEAT_Meal	93.9	57.6	4.2	0.51
MEAT_MeatBone	94	54.2	4.73	0.39
MOLASSES_Beet_Sugar	77.9	8.5	0.03	0.6
MOLASSES_Sugarcane	74.3	5.8	0.1	0.47
OATS_GrainRolled	90	13.2	0.4	0.19
OATS_Hay_headed	91.9	9.1	0.22	0.14
OATS_Silage_headed	34.6	12.9	0.31	0.19
PEANUT_Meal	92.3	51.8	0.64	0.32
POTATO_Byproduct_meal	35.4	10.5	0.29	0.11
RICE_Bran	90.6	15.5	1.78	0.19
RYE_ANNUAL_Silage_vegetative	29.7	16.1	0.42	0.2
SAFFLOWER_Meal	93.5	29	0.72	0.32

Table 9 continued

	Dry matter (%)	Crude protein (%)	Phosphorus (%)	Sulfur (%)
SORGHUM_GRAIN_TYPE_GrainRolled	88.6	11.6	0.35	0.11
SORGHUM_GRAIN_TYPE_Grain_steam-flaked	88.6	11.6	0.35	0.11
SORGHUM_GRAIN_TYPE_Silage	28.8	9.1	0.21	0.12
SORGHUM_SUDAN_TYPE_Hay	86.5	9.4	0.2	0.13
SORGHUM_SUDAN_TYPE_Silage	28.8	10.8	0.24	0.15
SOYBEAN_Hulls	90.9	13.9	0.17	0.12
SOYBEAN_Meal_expellers	89.6	46.3	0.66	0.34
SOYBEAN_Meal_nonenzymaticallyBrowned	50	27	0.75	0.4
SOYBEAN_Meal	89.1	49.9	0.71	0.46
SOYBEAN_Meal	89.5	53.8	0.7	0.39
SOYBEAN_Seeds_whole	90	39.2	0.6	0.31
SOYBEAN_Seeds_whole_roasted	91	43	0.64	0.32
SOYBEAN_Silage_early_maturity	40.4	17.4	0.37	0.22
SUNFLOWER_Meal	92.2	28.4	1	0.39
SUNFLOWER_Oil_seeds	91.8	19.2	0.51	0.21
TOMATO_Pomace	24.7	19.3	0.47	0.15
TRITICALE_Silage_headed	32	13.8	0.33	0.21
WHEAT_Bran	89.1	17.3	1.18	0.21
WHEAT_Grain_rolled	89.4	14.2	0.43	0.15
WHEAT_Hay_headed	86.8	9.4	0.2	0.13
WHEAT_Middlings	89.5	18.5	1.02	0.18
WHEAT_Silage_early_head	33.3	12	0.29	0.17
WHEAT_Straw	92.7	4.8	0.1	0.11
WHEAT_Wet_cattle	20.8	14.6	1.04	1.15

Sources of data:
Subcommittee on Dairy Cattle Nutrition and Committee on Animal Nutrition (2001), Maiga et al. (1997)

Appendix 3

See Table 10.

Table 10 Environmental factors parameterized in Manure-DNDC

1. Manure temperature in sheltered house	$T_{\text{house}} = T_{\text{air}} - 0.001 * VR * (T_{\text{air}} - 15)$ <p>where T_{house}, house temperature (°C); T_{air}, air temperature (°C); VR, ventilation rate (cubic meter/s)</p>
2. Temperature change in compost	$dT_{\text{compost}} = (H_{\text{gain}} - H_{\text{loss}}) \times 10^6 / M_{\text{compost}} / SHC_{\text{compost}};$ $H_{\text{gain}} = a * SHV_C * CO_{2\text{compost}};$ $H_{\text{loss}} = b * (T_{\text{compost}} - T_{\text{air}}) / M_{\text{compost}};$ <p>where dT_{compost}, daily temperature change in compost (°C); H_{gain}, heat gain due to organic C oxidation (MJ); H_{loss}, heat loss due to heat transfer from compost to air (MJ); $CO_{2\text{compost}}$, daily CO_2 flux produced in compost (kg C/day); M_{compost}, manure mass in compost (kg); SHC_{compost}, manure specific heat capacity (800–1,480 J/kg K); SHV_C, specific heating value of C oxidation (20 MJ/kg); a, constant coefficient; b, constant coefficient subject to coverage type of compost</p>

Table 10 continued

3. Temperature change in lagoon	$dT_{\text{lagoon}} = H_{\text{lagoon}} * 10^6 / M_{\text{lagoon}} / SHC_{\text{water}};$ $H_{\text{lagoon}} = k * (T_{\text{lagoon}} - T_{\text{air}}) * S_{\text{lagoon}} * F_{\text{cover}};$ <p>where dT_{lagoon}, daily temperature change in lagoon ($^{\circ}\text{C}$); H_{lagoon}, daily heat flux at interface between lagoon and air (MJ/day); T_{lagoon}, daily lagoon temperature ($^{\circ}\text{C}$); T_{air}, daily air temperature ($^{\circ}\text{C}$); M_{lagoon}, slurry mass (kg); SHC_{water}, specific heat capacity of water (4,187 J/kg K); S_{lagoon}, lagoon surface area (m^2); F_{cover}, factor of lagoon coverage (0–1); k, constant coefficient</p>
4. Water evaporation from compost	$EVA_{\text{compost}} = a * e^{(0.0585 * T_{\text{compost}})} * D_{\text{compost}} * W_{\text{compost}};$ <p>where EVA_{compost}, daily evaporation rate in compost (kg water/day); T_{compost}, compost temperature ($^{\circ}\text{C}$); D_{compost}, compost density (kg/m^3); W_{compost}, compost water content (kg water)</p>
5. Redox potential (Eh)	$Eh = Eo + RT/nF * \ln([O]/[W]),$ <p>where Eh, redox potential (volts); Eo, standard redox potential (volts); R, gas constant; T, temperature in kelvins; n, number of the electrons transferring in the redox reaction; F, Faraday constant; [O], concentration of oxidant (mol/L); [W], concentration of reductant (mol/L)</p>
6. Microbial growth rate	$GR = GR_{\text{max}} * DOC / (Ka + DOC) * [O] / (Kb + [O]),$ <p>where GR, growth rate; Rmax, maximum growth rate; DOC, concentrations of dissolved organic C; [O], concentrations of oxidant; Ka and Kb, half-saturation constants for substrates DOC and oxidant, respectively</p>

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