Comparison of process-based models to quantify nutrient flows and greenhouse gas emissions associated with milk production

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ABSTRACT

Assessing and improving the sustainability of dairy production systems is essential to secure future food production. This requires a holistic approach to reveal trade-offs between emissions of the different greenhouse gases (GHG) and nutrient-based pollutants and to ensure that interactions between farm components are taken into account. Process-based models are essential to support whole-farm mass balance accounting. How-

ever, since variation between process-based model results can be large, there is a need to compare and better understand the strengths and limitations of various models. Here, we use a whole-farm mass-balance approach to compare five process-based models in terms of predicted carbon (C), nitrogen (N) and phosphorus (P) flows and potential global warming impact (GWI) associated with milk production at the animal, field and farm-scale. We include two whole-farm models complemented by two field-scale models and one animal-based model. A whole-farm mass-balance framework was used to facilitate model comparison at different scales. GWIs were calculated from predicted emissions of methane (CH₄) and nitrous oxide (N₂O) and soil C change. Results show that predicted whole-farm GWIs were similar for the two whole farm models, ManureDNDC and IFSM, with a predicted GWI of 9.3 and 10.8 Gg CO₂eq. year⁻¹ for ManureDNDC and IFSM, respectively. Enteric CH₄ emissions were the single most important source of greenhouse gas emissions contributing 47% to 70% of the total farm GWI. Model predictions were comparable, that is, within a factor of 1.5, for most flows related to the animal, barn and manure management system. In contrast, predicted field emissions of N₂O and ammonia (NH₃) to air, N and P losses to the hydrosphere and soil C change, were highly variable across models. This indicates that there is a need to further our understanding of soil and crop N, P and C flows and that measurement data on nutrient and C flows are particularly needed for the field. In addition, there is a need to further understand how anaerobic digestion influences manure composition and subsequent emissions of N₂O and NH₃ after application of digestate to the field. Empirical data on manure composition before and after anaerobic digestion are essential for model evaluation.

Keywords: nutrient flows; greenhouse gas (GHG) emissions; process-based models; milk production; whole-farm mass-balance

1. Introduction

The livestock production sector is a key contributor to environmental challenges at local, regional and global scales (Steiner et al. 2006, Pelletier and Tyedmers, 2010, Bouwman et al. 2013). Ruminant livestock systems

contribute to global warming through greenhouse gas (GHG) emissions. The global dairy sector is reportedly responsible for 2.7% of global GHG emissions (FAO, 2010). In the US, the dairy sector is responsible for approximately 1.9% of GHG emissions (Thoma et al. 2013). In addition, crop-livestock production systems are the largest cause of human alteration of global nitrogen (N) and phosphorus (P) cycles (Bouwman et al. 2013), with repercussions for human health (e.g. secondary particle formation due to ammonia (NH_3) emission and drinking water contamination by nitrate (NO_3^-)) and the environment (e.g. eutrophication of lakes and coastal waters and exacerbation of hypoxic zones) (Schindler et al. 2008; Davidson et al. 2012). Finally, P is a limited resource, and sustaining an adequate P supply is a major emerging challenge (Cordell and White, 2014).

Assessing and improving the sustainability of dairy production is essential to secure future food production. This is, however, challenging for several reasons. First, in nonhomogeneous countries like the US, milk production practices and climatic conditions vary widely, which can result in large farm-specific variations in GHG emissions and nutrient losses (Del Grosso et al. 2005; Henderson et al. 2013). Second, in dairy production systems, N, P and carbon (C) flows are interrelated. Consequently, mitigation of one pollutant can increase emissions of another pollutant. For example, Dijkstra et al. (2011) suggested that dietary strategies that reduce N excretion from dairy cows may increase enteric methane (CH_4) emissions. Third, nutrient flows between farm components, such as the animal herd, the manure management system, the field, and the feed, are strongly linked. Altering one component of this nutrient cycle can have major effects on nutrient flows to or from other farm components.

Understanding trade-offs between emissions of GHGs and nutrients ensures that interactions between N, P and C cycling and farm components are considered in management decisions. Commonly used sustainability assessment methodologies such as life cycle assessment (LCA) often employ Intergovernmental Panel on Climate Change (IPCC) Tier 1 emission factors to quantify nutrient and GHG emissions. These emission factors are often based on rough emissions estimates and cannot account for temporally and spatially-explicit variations. IPCC Tier 2 methods are more advanced, particularly for livestock, and GHG emissions can be predicted based on animal activity data, diet characteristics and livestock type. This provides a more spatial-explicit characteri-

zation of these flows. However, IPCC methods were primarily developed to quantify GHG emissions rather than to quantify flows of N- and C-based compounds. Also, as there are no P-based GHGs, the IPCC methods are not directly applicable to quantify P losses. Thus, IPCC Tier 1 and Tier 2 methods neither consider nutrient cycling between different farm components nor account for interactions between N, P, and C flows. From a sustainability perspective this may mask nutrient and carbon imbalances, resulting in unaccounted nutrient and/or carbon losses or gains at animal, field or farm scales. Reliance on IPCC Tier 1 or Tier 2 methods may also result in sub-optimal improvements when trade-offs occur. Finally, it is generally thought that the environmental performance of dairy farms can be improved by improving nutrient cycling efficiency across farm components, and subsequently reducing nutrient losses.

A whole-farm, holistic approach explicitly considers nutrient cycling across farm components (e.g., Schils et al. 2005, Schils et al. 2007). It includes a mass-balance analysis that considers nutrient imports to the farm, exports from the farm, and internal nutrient flows between farm components. It is a powerful methodology to develop GHG mitigation strategies for farming systems (e.g., Schils et al. 2005, Schils et al. 2007, del Prado et al. 2013). Parameterization of a whole-farm mass-balance is challenging because it is difficult, relatively inaccurate, and expensive to measure the assimilation and emission of GHGs and to empirically determine internal nutrient flows at the whole-farm scale (Rotz et al., 2010). Process-based models can predict flows when empirical data are lacking (e.g. Del Grosso et al. 2005, Schils et al. 2005, Li et al. 2012). In addition, process-based models can account for underlying processes influencing N, P, and C flows, and may yield more reliable results than emission factors (e.g. Del Grosso et al. 2005, Schils et al. 2005, Li et al. 2012). A whole-farm approach may thus be particularly powerful when process-based models are used to predict emissions and internal flows simultaneously. Variation between process-based model results may, however, be large. Thus, there is a need to compare and understand the strengths, limitations, and concordance of various models.

In response to these needs, we performed a quantitative comparison of five process-based models in terms of predicted N, P and C flows and predicted GWIs for a commercial dairy farm in New York State. We included two whole-farm models, two field models, and one animal model. The objective was to i) compare models in

terms of predicted N, P and C flows and GWI associated with six farm components (animal, barn, manure storage, soil, crop and feed), and to *ii*) analyse the level of concordance between the models and identify needs for improvement. We focused our comparison on predicted emissions of CH₄, N₂O and NH₃ to air and N and P losses to the hydrosphere. Methane and N₂O are GHGs contributing to global warming, NH₃ is a criteria air pollutant, and N and P losses to the hydrosphere contribute to eutrophication and the exacerbation of hypoxic zones. This model comparison study provides a basis for evaluating GHG mitigation and nutrient efficiency optimization strategies and is part of a larger project that aims to reduce the life cycle environmental impact of dairy production systems in the US (www.sustainablemilk.org). The output of the process-based models will be used to inform sustainability assessment methodologies such as LCA. A follow-up project will focus on (partial) model evaluation with field measured data.

2. Methods

2.1 General approach

An overview of the whole-farm mass-balance framework and the farm components, processes and environmental emissions considered is provided in Figure 1. Process-based models operating at different scales were included. To ensure a fair and consistent comparison, *i*) all models were setup using similar input data to represent the same dairy farm, and *ii*) a whole-farm mass-balance framework was used to compare model predictions of N, P and C flows and GWPs per farm component (animal (three models), barn (two models), manure management (two models), soil (four models) and crops (four models)).

2.2 Modelled farm

The modelled farm is a commercial dairy farm in central New York, as managed in 2009. Input data collected include herd characteristics, detailed feed scenarios per animal group, crop cultivation practices, a description of the manure management system, soil characteristics, and representative weather data. A more detailed description of farm characteristics is in the Supporting Information (SI). The farm had 1096 lactating cows, 165 dry cows and 1340 replacement animals, including 250 heifer calves (SI, Table S2). Annual average milk production

122 was 10,394 L cow⁻¹. A small percentage of milk was fed to heifer calves, while the rest (10,263 L cow⁻¹ year⁻¹),
123 was sold. In addition to milk, 600 animals (300 calves and 300 cows), 90.7 metric tons of manure solids, and
124 564 metric tons of wheat were exported from the farm (SI, Table S1, S8 and S9). Animals were housed in two
125 free-stall barns (SI, Table S12). Manure was collected continuously from the barns by an automated scraper,
126 into a reception pit and transferred to an anaerobic digester. The digestate leaving the digester was run
127 through a solids separator, whose solids were partly used as bedding in the barns. The remaining solids were
128 sold off farm or applied to cropland on farm. The separated liquid from the digester was stored in a lagoon and
129 applied on cropland.

130 Crops were cultivated on 982 hectares of land. Soil information was retrieved from the Soil Survey Geo-
131 graphic (SSURGO, websoilsurvey.nrcs.usda.gov) database according to the dominant soil series, a Honeoye silt
132 loam (fine-loamy, mixed, mesic Glossoboric Hapludalfs) with 5% slopes (SI, Table S15). Corn (*Zea mays* L.), win-
133 ter wheat (*Triticum aestivum* L.), alfalfa (*Medicago sativa* L.) and grass were grown on the farm. Corn, winter
134 wheat, and alfalfa were grown in an 8-year rotation with three years corn, one year wheat, and four years alfa-
135 fa. A crop rotation schedule was developed based on hectares provided by the farmer and the USDA Crop Data
136 Layer (http://www.nass.usda.gov/Research_and_Science/Cropland/Release/) for the 2008-2013 period (SI, Ta-
137 ble S11). In total, 66.5% of cropland was used for the 8-year rotation cycle and 33.5% for continuous corn si-
138 lage, corn grain, and grass. The rotated cropland was split into eight sub-areas so that each crop was present
139 every year. Overall, alfalfa, corn silage, corn grain, wheat and grass were grown on 33%, 29%, 25%, 8% and 5%
140 of the cropland, respectively. The farm produced 78% of the total animal feed. Supplemental protein and min-
141 eral feeds were purchased (SI, Table S5). Detailed animal feed rations per animal group are listed in Table S3
142 and S4. A field management schedule was developed based on data obtained on fertilizer and manure applica-
143 tion rates, manure composition (SI, Table S14), general application dates (e.g. 'spring' application), and crop
144 planting dates (SI, Table S12 and S13).

145 Historical weather data representative of the farm was obtained from the North American Regional Reana-
146 lysis (<http://www.esrl.noaa.gov/psd/data/gridded/data.narr.html>). This provided daily maximum and minimum

147 temperature, precipitation, wind speed, and relative humidity, while solar radiation was estimated using the
 148 APEX model (Williams et al., 2012; version 0806).

149 Collected farm data were used as model inputs (see below) and also to derive empirical nutrient flows,
 150 which were compared to model predictions. Empirically-derived flows were expressed in a common unit, i.e. kg
 151 N per year and kg P per year. Nitrogen and P contents in milk, meat, purchased feed and harvested crops were
 152 calculated according to Soberon et al. (2013). A detailed description on data conversions is provided in the
 153 Supporting Information. The empirical nutrient flows are in Table 1.

154 Following Soberon et al. (2013), we calculated whole farm nutrient mass-balances (NMB) for N and P as the
 155 amount of nutrients imported onto the farm (nutrients in feed, fertilizer, animals and bedding) minus the
 156 amount of nutrients exported from the farm (nutrients in milk, animals, crop and manure) per tillable hectare.
 157 This gives an NMB of 103 and 15 kg nutrient ha⁻¹ for N and P, respectively (Table 1). This is comparable to, al-
 158 though slightly higher than, the benchmark for current NY dairy farms (NMB-N = 118 kg N ha⁻¹, and NMB-P = 13
 159 kg ha⁻¹ (Cela et al. 2014). The positive NMBs indicate a surplus of nutrients on the dairy farm, which can be lost
 160 to the environment.

161 **Table 1. Empirically-derived nutrient flows for the NY dairy farm**

Flow characteristic	N (kg N yr ⁻¹)	P (kg P yr ⁻¹)
Import		
Feed	154,892.77	25,147.17
Fertilizer	27,062.44	4,215.54
Animals	0	0
Export		
Milk	67,694.35	11,648.26
Animals	5,878.56	1,415.21
Crops	6,576.06	1,495.49
Manure	616.89	99.79
Internal		
Crops produced (excl. cash crops)	194,008.77	26,587.55
Animal feed intake	336,614.01	49,236.90
Feed storage	3,43.97	401.34
Manure application on field	119,894.94	49,236.90
Whole farm	N (kg N ha⁻¹)	P (kg P ha⁻¹)

NMB	103	15
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2.3. Model description

The model comparison included two whole-farm models (ManureDNDC and IFSM 4.2), one animal model (CNCPS 6.1.54) and two field models (APEX 0806 and DayCent 4.5). All models are well-established and have been partially evaluated with empirical data for different farm components (e.g. *IFSM*: Rotz et al. 1999, Rotz et al. 2006, Rotz et al. 2014, *Manure-DNDC*: Deng et al. 2015, Li et al. 2012, Giltrap et al. 2010, *CNCPS*: Higgs et al. 2012, Higgs et al. 2013, *APEX*: Gassman et al. 2010, *DayCent*: Jarecki et al. 2008, Del Grosso et al. 2008a). Each model has unique features, as briefly described here.

Manure-DNDC (www.dndc.sr.unh.edu/) provides a detailed description of the on-farm biochemical cycle of N and P as well as the use of water for individual crops (alfalfa, corn, grass and winter wheat). The model can predict crop growth, soil temperature and moisture regimes, soil C dynamics, N leaching, and emissions of trace gases including nitrous oxide (N₂O), nitric oxide (NO), dinitrogen (N₂), ammonia (NH₃), methane (CH₄) and carbon dioxide (CO₂). A specific feature of DNDC is its biogeochemical model for quantifying greenhouse gas and NH₃ emissions from manure systems (Li et al. 2012). The current version of ManureDNDC does not have a nutrition module (Li et al. 2012). Instead, empirical relationships and/or fixed emission factors are used to quantify animal-related flows such as rumen CH₄ production, enteric N₂O emission, and N, P and C in milk production (Li et al. 2012).

The Integrated Farm System Model (IFSM), (<http://www.ars.usda.gov/Main/docs.htm?docid=8519/>) simulates the performance, economics and environmental impacts of farm production systems (Rotz et al., 2012). IFSM provides emissions for all major farm components including individual crops, machinery, cattle and manure sources. IFSM uses a range of methods to quantify emissions, including process simulation and process related empirical relationships, and emission factors for simple processes.

The *Cornell Net Carbohydrate and Protein System (CNCPSv6.1 www.cncps.cornell.edu/)* is an animal model that predicts changes in NH₃ and CH₄ emissions for a wide range of feed, environmental and ration characteris-

185 tics (Tylutki et al. 2008, Van Amburgh et al. 2010, Higgs et al. 2012, Higgs et al. 2013). The model provides en-
 186 teric emissions and nutrient balances on a per cow basis.

187 *DayCent* (www.nrel.colostate.edu/) is a daily-time step, plant-centric soil biogeochemical model (Del Grosso
 188 et al. 2001, 2002, 2005). Model outputs include daily fluxes of various N-gas species (e.g., N₂O, NO_x, N₂), dai-
 189 ly CO₂ flux from heterotrophic soil respiration, soil organic C stock changes, net primary productivity (NPP), dai-
 190 ly water and nitrate (NO₃) leaching, and other ecosystem parameters.

191 *APEX* (Williams et al. 2012, www.epicapex.tamu.edu/) is a comprehensive, daily-time step model able to link
 192 field to watershed-scale processes, simulating detailed agricultural management impacts and vegetation prod-
 193 uctivity as well as a suite of environmental processes including hydrology, erosion, net ecosystem exchange,
 194 soil carbon dynamics and nitrogen balance (Gassman et al., 2010).

195 **Table 2. Coverage of the considered process-based models in terms of farm component, nutrient flows and**
 196 **GHG emissions.**

	IFSM	Manure- DNDC	CNCPS	APEX	DayCent
Model scale	Whole-farm	Whole-farm	Animal	Field	Field
Animal					
Milk & meat production	N, P, C	N, P, C	n.a.		
Manure excreted	N,P, C	N,P,C	N, P		
Respiration	CO ₂ -C	CO ₂ -C	n.a.		
Enteric	N ₂ O-N, CH ₄ -C	N ₂ O-N, CH ₄ -C	CH ₄ -C		
Barn					
Ammonia volatilization	NH ₃ -N	NH ₃ -N			
Manure from barn to ma- nure management	N,P,C	N,P,C			
Other barn emissions	N ₂ O-N, N ₂ -N, NO-N, CH ₄ -C	N ₂ O-N, N ₂ -N, NO-N, CH ₄ -C			
Manure management (anaerobic digester + lagoon)					
Manure exported from farm	N,P,C	(N, P, C)*			
Emissions to air	NH ₃ -N, N ₂ O- N, N ₂ -N, NO- N, CH ₄ -C, CO ₂ -C	NH ₃ -N, N ₂ O- N, N ₂ -N, NO- N, CH ₄ -C, CO ₂ -C			
Field processes					
Crop yield	N, P, C	N, P, C		N, P, C	N, P, C
Cash crops	N,P,C	(N, P, C)*			
(De)nitrification	N ₂ O-N, NO-	N ₂ O-N, NO-		N ₂ O-N, N ₂ -N	N ₂ O-N, NO-

	N, N ₂ -N	N, N ₂ -N		N, N ₂ -N
Ammonia volatilization	NH ₃ -N	NH ₃ -N	NH ₃ -N	NH ₃ -N **
Methane emission	CH ₄	CH ₄	n.a.	CH ₄
Run-off	N,P,C	N,P,C	N,P,C	n.a.
Leaching	N,P,C	N,P,C	N,P,C	N,P,C
Erosion	N,P,C	n.a.	N,P,C	n.a.
CO ₂ assimilation	CO ₂ -C	CO ₂ -C	CO ₂ -C	CO ₂ -C
Soil C change	C	C	C	C
N fixation	N	N	N	N
Soil accumulation	P	P	P	P

n.a. = not available, i.e., the model does not simulate this process. * This is a mass-balance estimate. ** DayCent predicts NH₃ volatilization from harvested and senesced biomass N and does not predict NH₃ volatilization from manure application (further details described below).

2.4. Model simulation

All models were set up to simulate the commercial dairy farm in New York State. All models except CNCPS simulated at least eight years to represent the specified crop rotation cycle. ManureDNDC was modified to accommodate the eight year crop rotation cycle. Modifications included an incorporation of 'carry-over' of manure from one year to the next in the lagoon and digester. ManureDNDC simulations were run for 9 years (8 years to accommodate the crop rotation cycle and a 1 year spin-up). IFSM simulations were run for 25 years and the average annual model output was used to obtain typical N, P, C flows. For IFSM, no spin-up phase is used. For DayCent and APEX a 20 year (1980-1999) spin-up phase was used. Both models were run from 1980 to 2013 and model outputs from 2000 to 2013 were averaged to obtain typical N, P and C flows.

Table 2 provides an overview of the respective N, P and C flows considered by each model that are relevant to this study. All these flows are model predictions as opposed to user-defined inputs. Regarding the model inputs, it should be mentioned here that the two whole-farm models require different inputs. ManureDNDC requires daily feed rations, including quantity and characteristics, as an input to the model. IFSM contains an animal sub-model that predicts all feed and purchased feed supplements needed to meet the protein and energy requirements of all animals. IFSM was set-up in such a way, that feed inputs would match the empirically-derived feed rations as close as possible. Purchased feed supplements, as used in IFSM, are based on the empirically-derived feed rations. Both IFSM and ManureDNDC were set-up to match the manure

application rates to the field, and the amount of manure solids used as bedding material, as derived from the manure management plan, as close as possible. Manure export flows and N, P, and C content in this flow, were predicted based on mass-balance considerations by both models. Feed supplements were considered to be purchased, representing an N, P and C import to the farm. This flow was quantified based on the empirical data. For ManureDNDC, a mass-balance approach was used to quantify the amount of N, P and C in cash crops and/or additional feed purchases. That is, the amount of N, P, and C in cash crops or added feed purchases were calculated as the difference between N, P, and C content in predicted crop yield and the N, P and C content of feed rations (empirical data). IFSM cash crop exports were determined from harvested yield and assigned nutrient concentrations in the grain (NRC, 2001).

The field models APEX and DayCent require manure application rates as an input. The manure N-application to the field, as derived from the manure management plan, indicated an unrealistically large loss of N during manure storage. This was supported by IFSM and ManureDNDC simulations, which predicted higher manure N application rates to the field based on the scale of farm production. To ensure comparability of model inputs, we therefore adjusted the manure application rates for the field models APEX and DayCent to align with IFSM predicted manure application rates per crop.

While field application of manure contributes substantially to whole-farm NH_3 emissions, the field emissions predicted by DayCent only represent NH_3 volatilization of a plant-specific portion of harvested or senesced biomass N (del Grosso et al. 2008b). At present, DayCent does not simulate NH_3 volatilization from manure application on the field, whereas this process is simulated in the other models. To ensure a consistent comparison, the potential amount of N lost due to NH_3 volatilization was subtracted from the total amount of N in manure applied to the field in DayCent simulations. The potential amount of NH_3 -N volatilized was obtained from IFSM simulations. This provided the amount of manure N incorporated into the soil used in DayCent simulations.

2.5 Global warming impact

241 In addition to a comparison of N, P, and C flows, we quantified the total global warming impact (total GWI)
 242 of the farm by multiplying the emissions of CH₄ and N₂O with the substance-specific global warming potential
 243 (GWP₁₀₀ including carbon-cycle feedback; 1 kg CO₂-eq kg CO₂⁻¹, 34 kg CO₂-eq kg CH₄⁻¹ and 298 kg CO₂-eq kg N₂O⁻¹;
 244 ¹; IPCC, 2013) to yield total global warming potentials in CO₂ equivalents. We also included the potential global
 245 warming impact (positive or negative) associated with soil C change in our calculation of the total GWI. This
 246 was done by converting predicted changes in soil C content to CO₂ and multiplying by the GWP for CO₂. Other
 247 biogenic CO₂ emissions were excluded from the quantification of total GWI as the remaining CO₂ fixed by plant
 248 photosynthesis is eventually returned to the atmosphere as respired CO₂ by microorganisms, animals and hu-
 249 mans when considering the entire life cycle of dairy products (IPCC, 2006, Ch.10). Similar to nutrient related
 250 emissions, GHG emissions and potential GWIs were allocated to each of the five main farm components consi-
 251 dering only the relevant outputs for each model. For the field, GHG emissions and GWIs were also allocated to
 252 specific crops. Agricultural soils can contribute to indirect N₂O emissions, via two pathways: 1) following NH₃
 253 and NO_x volatilization and the subsequent re-deposition of reactive nitrogen on soils and surface waters and 2)
 254 through leaching and runoff of NO₃, which is converted into N₂O in streams and waterways (IPCC, 2006. Ch.
 255 11). Presently, none of the included models predicts these indirect N₂O emissions and we therefore did not in-
 256 clude them in our model comparison. However, IPCC (2006, Ch. 11) provides emission factors to estimate indi-
 257 rect N₂O emissions from NH₃ and NO emissions (EF = 0.010 kg N₂O-N/kg NH₃-N or kg NO-N emitted) and NO₃
 258 losses (EF = 0.0075 kg N₂O-N/kg NO₃-N lost). These emission factors were used to estimate the contribution of
 259 indirect N₂O emissions to the potential global warming impact.

260 **3. Results and discussion**

261 **3.1 Model comparison – animal, barn, manure management**

262 Model predictions were comparable, that is within a factor of 1.5, for most nutrient and carbon flows re-
 263 lated to the *animal and the barn* including N and P in milk and meat production, N, P and C excreted in manure,
 264 CO₂ respiration, NH₃ volatilization and manure N, P and C removal from the barn to the manure management

265 system (Fig. 2^{b,c} – 4^{b,c}, Table 3). For N and P in milk produced, model predictions of the whole-farm model IFSM
 266 were very similar to the empirically-derived number for the modelled farm, at 69,651 kg N yr⁻¹ and 67,594 kg N
 267 yr⁻¹ for N, and 11,647 kg P yr⁻¹ and 11,648 kg P yr⁻¹ for P, respectively (Table 3). ManureDNDC predicted a lower
 268 amount of N and P in milk produced, i.e. 45,678 kg N yr⁻¹ and 9,822 kg P yr⁻¹, respectively. These estimates dif-
 269 fered by less than a factor of 1.5 from IFSM predictions and the empirically-derived number (Table 1,3; Fig. 2^{a-c};
 270 3^{a-c}). For C, ManureDNDC predicted a considerably lower export with milk compared to IFSM, i.e. 182,713 kg C
 271 yr⁻¹ and 835,527 kg C yr⁻¹ for ManureDNDC and IFSM, respectively. ManureDNDC does however allocate a larg-
 272 er carbon flow to manure excreted and meat produced (Table 3, Fig. 4^{b,c}). Based on an average composition of
 273 raw milk (major C containing compounds only: 4.6% casein, 4.9% lactose, 1% palmitic acid, 0.4% myristic acid,
 274 0.4% stearic acid), we estimated a C:N ratio in produced milk of approximately 9 (SI Table S22, S23). The pre-
 275 dicted C:N ratio by IFSM is ~12 and the predicted C:N ratio by ManureDNDC is ~4 (Table 3), suggesting that
 276 ManureDNDC incorrectly predicts a too low milk C content, whereas IFSM slightly overestimates milk C con-
 277 tent. At present, ManureDNDC does not have a nutrition module and a combination of empirical relationships
 278 and fixed emission factors are used to predict N, P and C in milk production (Li et al. 2012). Our results indicate
 279 that this approach can underestimate N, P and C flows in milk production for specific feed rations, particularly
 280 for C.

281 In terms of NH₃ emissions, simulated barn emissions were within a factor of 1.2 for IFSM and ManureDNDC
 282 (Table 3, Fig. 2^{b,c}). This was not unexpected as comprehensive field evaluation studies have shown both models
 283 to accurately predict barn NH₃ emissions both in terms of temporal trend and magnitude (Rotz et al. 2014; Li et
 284 al. 2012; Deng et al. 2015). These evaluation studies were partly performed with empirical data measured on
 285 the simulated NY dairy farm (Rotz et al. 2014; Deng et al. 2015). As part of the National Air Emissions Monitor-
 286 ing Study (NAEMS) program, Bogan et al. (2010) measured NH₃ emissions in one of the two barns on the farm.
 287 The yearly average observed NH₃ emission was 43.2 g NH₃ cow⁻¹ day⁻¹ for a barn with 470 lactating cows. To
 288 compare this empirical observation with the predicted barn NH₃ emissions for the entire farm, these measured
 289 data were adjusted to 500 kg animal units, which corresponded to the average weight of all animals on the NY

290 farm. This results in an empirical average NH_3 emission of $34 \text{ g NH}_3 \text{ AU}^{-1} \text{ day}^{-1}$. Predicted barn ammonia emis-
291 sions for IFSM ($25 \text{ g NH}_3 \text{ AU}^{-1} \text{ day}^{-1}$) and ManureDNDC ($30 \text{ g NH}_3 \text{ AU}^{-1} \text{ day}^{-1}$) were within a factor of 1.4 of the
292 observed value and correspond well with the empirical data.

293 In terms of greenhouse gas emissions, predicted enteric CH_4 emissions were similar for IFSM and CNCPS at
294 0.17 and $0.20 \text{ Gg CH}_4\text{-C yr}^{-1}$ (0.22 and $0.27 \text{ Gg CH}_4 \text{ yr}^{-1}$), respectively (Table 3). ManureDNDC predicted a lower
295 enteric CH_4 emission of $0.10 \text{ Gg CH}_4\text{-C yr}^{-1}$ ($0.13 \text{ Gg CH}_4 \text{ yr}^{-1}$), however, ManureDNDC predicted a higher emis-
296 sion of CH_4 from the barn floor (in comparison to IFSM) and the total CH_4 emission of the animal and housing
297 facility together was equal to IFSM predictions (Fig. 4^{a,b}).

298 **Table 3. Comparison of predicted N, P and C flows**

299

Process	IFSM	Manure-DNDC	APEX	DayCent	CNCPS	Ratio (max. /min.)	Empirical data
Model scale	Whole farm	Whole farm	Field	Field	Animal		
Production							
Animal							
N in milk produced (kgN yr ⁻¹)	69,651.0	45,678.0				1.5	67,594.4
P in milk produced (kgP yr ⁻¹)	11,647.0	9,822.0				1.2	11,648.3
C in milk produced (kgC yr ⁻¹)	835,527.0	182,713.0				4.6	
N in meat produced (kgN yr ⁻¹)	10,203.0	28,172.0				2.8	5,878.6
P in meat produced (kgP yr ⁻¹)	2,931.0	3,395.0				1.2	1,415.21
C in meat produced (kgC yr ⁻¹)	84,560.0	102,445.0				1.2	
Field							
Crop yield N (kgN yr ⁻¹)	183,414.0	154,455.8	162,154.0	202,730.5		1.3	194,008.8
Crop yield P (kgP yr ⁻¹)	20,497.0	7,104.6	18,543.9	22,895.4		3.2	26,587.55
Crop yield C (kgC yr ⁻¹)	3,308,778.0	3,974,509.6	3,682,145.1	4,152,309.2		1.3	
Environmental emissions							
Animal							
Enteric N ₂ O emission (kgN yr ⁻¹)	158.0	3.0				52.7	
Enteric CH ₄ emission (kgC yr ⁻¹)	167,110.0	96,144.0			199,565.9	2.1	
Barn							
NH ₃ emission (kgN yr ⁻¹)	18,063.0	21,767.4				1.2	
Other barn emissions - N ₂ O (kgN yr ⁻¹)	0	1,956.8				>>	
Other barn emissions - CH ₄ (kgC yr ⁻¹)	2,924.0	74,761.6				25.6	
Manure management							
NH ₃ emission (kgN yr ⁻¹)	16,029.0	10,129.0				1.6	
N ₂ O emission (kgN yr ⁻¹)	285.0	318.6				1.1	
CH ₄ emission (kgC yr ⁻¹)	26,541.0	39,255.0				1.5	
Field							
Nitrification + denitrification - N ₂ O (kgN yr ⁻¹)	2,846.3	257.4	1,148.4	6,132.4		23.8	

NH ₃ emission (kgN yr ⁻¹)	42,546.0	126,624.9	23,062.4	3,842.1*	5.5
Leached N loss (kgN yr ⁻¹)	58,530.2	70,946.3	44,670.1	91,492.8	2.0
Runoff N loss (kgN yr ⁻¹)	982.0	0	12,907.9	n.a.	>>
Erosion N loss (kgN yr ⁻¹)	67.0	0	14,203.4	n.a.	>>
Leached P loss (kgP yr ⁻¹)	24.0	283.5	78.5	20.6	13.7
Runoff P loss (kgP yr ⁻¹)	108.0	10.9	403.2	n.a.	37.1
Erosion P loss (kgP yr ⁻¹)	592.0	0.0	3,090.1	n.a.	>>
Soil P accumulation (kgP yr ⁻¹)	9,108.0	25,982.5	12,523.5	11,685.4	2.9
CH ₄ emission (kgC yr ⁻¹)	321.0	-585.0	n.a	1,027.4	>>
Soil C change (kgC yr ⁻¹)	0.0	629,300.8	-683,967.4	8,877.7	>>

*Note that DayCent predicts NH₃ volatilization from harvested and senesced biomass N and does not predict NH₃ volatilization from manure application.

303 The main difference between the two whole-farm models relates to predicted N₂O emissions from the
304 barn floor (Table 3, Fig. 2^{a,b}). ManureDNDC predicted a N₂O emission close to 2,000 kg N for N₂O emissions
305 from manure on the barn floor, whereas IFSM simulated barn N₂O emissions were negligible. This difference is
306 attributable to a difference in model assumptions. In IFSM, N₂O emissions from manure are negligible when
307 manure is removed from the barn within a few hours of excretion, which is supported by limited measure-
308 ments of N₂O emissions in a free stall barn (Chianese et al. 2009). The rationale is that manure does not stay in
309 the barn long enough for substantial nitrification and denitrification processes to occur. An evaluation of Ma-
310 nureDNDC with limited observational data showed that modeled N₂O fluxes were in agreement with field mea-
311 surements for a free stall barn (Li et al. 2012). While this may indicate that ManureDNDC is capable of predict-
312 ing total N₂O emissions in the barn, it does not provide information on the importance of manure N₂O
313 emissions in comparison to enteric N₂O emissions. A further investigation of the relevance of manure N₂O
314 emissions in free stall barns where manure is removed shortly after excretion is needed. This appears impor-
315 tant as, according to ManureDNDC, barn N₂O emissions can contribute substantially to the whole-farm global
316 warming impact (see further below).

317 ManureDNDC and IFSM both predict enteric N₂O emissions. These predictions are based on limited empiri-
318 cal data indicating that a small amount of enteric N₂O is emitted by animals (Kaspar and Tiedje, 1981; Hamilton
319 et al. 2010). ManureDNDC and IFSM deviate substantially in their predictions of enteric N₂O, i.e. 3.0 kg N yr⁻¹
320 versus 158 kg N yr⁻¹ for ManureDNDC and IFSM, respectively (Table 3). However, as enteric N₂O emissions con-
321 tribute minimally to total farm N₂O emissions (Table 3) and the whole-farm global warming impact (see below),
322 improving model simulations of enteric N₂O emissions is of relatively low priority.

323 For the *manure management* system, predicted nutrient-related emissions were highly comparable be-
324 tween IFSM and ManureDNDC (Fig. 2^{b,c} – 4^{a,b}, Table 3). A minor exception was the predicted emission of N₂.
325 Predicted N₂ emissions were 3 times higher in ManureDNDC than in IFSM. From an environmental perspective,
326 this difference is irrelevant as N₂ is a natural, non-reactive component of the atmosphere. This loss of N does,
327 however, affect the whole farm balance and can, eventually, have an economic impact.

328 3.2 Model comparison – field

329 Comparing all models on a *field* scale shows that predictions of N, P and C harvested with crops were simi-
330 lar to each other for most models, except for the crop P yield predicted by ManureDNDC (Table 3, Fig. 2-4). The
331 crop P yield as predicted by ManureDNDC was one third that predicted by IFSM and the empirically-derived da-
332 ta, which resulted in a large import of P via purchased feed in ManureDNDC simulations to meet animal re-
333 quirements. All other predictions of crop nutrient yields were comparable, that is within a factor 1.3, to the
334 empirically-derived crop yield for the NY farm.

335 There is a considerable difference in predicted N fixation, with predictions ranging from 69,392 kg N yr⁻¹
336 (APEX) to 149,678 kg N yr⁻¹ (ManureDNDC). This impacts the field N balance and results in a substantially larger
337 predicted N accumulation in soil and N leaching loss from the alfalfa field by ManureDNDC in comparison to
338 the other models (Table 3, SI Table 16). Although all model simulations were performed using the same weath-
339 er data, small differences in N concentration in rainfall and differences in simulated years, resulted in deviating
340 predictions of N deposition (Fig. 2). The predicted difference is, however, small, in comparison to other N in-
341 puts such as manure application and fertilizer application, and does not have a large impact on the overall field
342 N balance. Field P and C inputs were comparable, that is within a factor of 1.1, across models (range P: 33,381 –
343 35,090 kg P yr⁻¹, range C: 7,330,234 – 8,136,170 kg C yr⁻¹) (Fig. 2-4).

344 Comparing all models in terms of environmental emissions, showed that *field* N,P,C flows were much more
345 variable across models than N,P,C flows associated with the animal, barn and manure management system
346 (Table 3). Nitrogen loss via NH₃ volatilization ranges from 23,062 kg N (APEX) to 126,625 kg N (ManureDNDC).
347 DayCent simulations were not included in this comparison as DayCent did not simulate NH₃ volatilization from
348 manure application on the field. Compared to the other models, ManureDNDC predicted very high NH₃ volatili-
349 zation from soil. In contrast, ManureDNDC underpredicted soil N₂O emissions compared to the other models
350 (257.4 kg N₂O-N yr⁻¹ (ManureDNDC) – 6,132.4 kg N₂O-N yr⁻¹ (DayCent)). These differences result from predicted
351 changes in the manure composition due to anaerobic digestion by ManureDNDC. During anaerobic digestion,
352 temperature-dependent hydrolysis reactions convert stable organic matter into more easily degradable C com-

353 pounds that are used for energy production. As a consequence, the amount of easily degradable C compounds
354 added to the soil upon manure application is reduced, which in turn reduces denitrification rates and thus N₂O
355 emissions. In addition, while the manure organic C transforms to dissolved organic carbon, CO₂ or CH₄, the or-
356 ganic N transforms to NH₄ (Li et al. 2012). Upon field application of manure, this increased amount of NH₄-N is
357 partially converted to ammonia, which causes a higher ammonia volatilization rate and a lower N₂O emission
358 rate as less NH₄ is available for nitrification and subsequent denitrification. The effects of anaerobic digestion
359 on organic C pools in manure are presently not simulated by APEX and DayCent. IFSM removes digested C via
360 CO₂ and CH₄ generated during anaerobic digestion from the manure but it does not simulate differences in the
361 forms (i.e. stability) of organic C. Exclusion of the digester from the manure management system (lagoon only)
362 results in a higher predicted N₂O emission by ManureDNDC of 901.5 kg N₂O-N yr⁻¹, which is more comparable
363 to emission estimates by IFSM (lagoon only, 2924 kg N₂O-N yr⁻¹), although still lower. At present, the effects of
364 anaerobic digestion on manure composition and emissions after field application are not well understood. In a
365 recent review on effects of anaerobic digestion on environmental emissions, Möller (2015) concluded that “the
366 direct effects of anaerobic digestion on field level emissions (NH₃- and N₂O- emissions, NO₃ - leaching) are neg-
367 ligible or at least ambiguous”. For N₂O, “most findings indicate a reduction of the soil-borne N₂O emission after
368 application of digestates in comparison to the undigested feedstocks, however the effects are influenced by
369 several environmental conditions, incl. soil water content, soil type and soil organic matter content” (Möller,
370 2015).

371 The models differed substantially in their prediction of *field* CH₄ emissions. Predicted field CH₄ emissions
372 range from -585 (ManureDNDC) to 1,027.4 kg C yr⁻¹ (DayCent). These field CH₄ emissions contributed negligibly
373 to the whole-farm CH₄ emissions and to the total global warming potential of the farm (see further below). Im-
374 proving model simulations of field CH₄ emissions is therefore of relatively low priority. At present, APEX does
375 not predict cropland CH₄ emissions.

376 For both N and P, there is large variability in predicted nutrient losses to the hydrosphere (Table 3, Fig. 2-3).
377 Overall, APEX predicted larger losses of N and P due to erosion and run-off than the other models. This differ-

ence is particularly striking for P. According to IFSM and APEX simulations, P losses from soil to groundwater and surface water mostly occur by erosion. There is, however, a relatively large difference, i.e. a factor of 5, in predicted erosion losses by these models. Erosion P losses range from 592 kg P yr⁻¹ for IFSM (0.6 kg P ha⁻¹ yr⁻¹) to 3090 kg P yr⁻¹ (3.1 kg P ha⁻¹ yr⁻¹) for APEX. Corn makes up most of the P erosion losses in both models with a P loss of 2,808 kg P yr⁻¹ (0.5 kg P ha⁻¹ yr⁻¹) and 477 kg P yr⁻¹ (2.8 kg P ha⁻¹ yr⁻¹) for IFSM and APEX, respectively. Comparing model predictions with field monitoring data of particulate P loss in the northern US, shows that IFSM predictions (0.6 kg P ha⁻¹ yr⁻¹) are comparable with the determined average particulate P loss of 0.3 kg P ha⁻¹ yr⁻¹ by Good et al. (2012) for a large set of agricultural fields with a broad range of management practices and field conditions as representative for Wisconsin. Consistently, Tomer et al. (2016) determined an annual average P loss of 1.0 and 1.8 kg P ha⁻¹ yr⁻¹ for a corn-corn-soybean rotation system in Iowa with and without annual fall (swine) manure application. APEX predictions are higher than the observed average value for particulate P loss, however, they are within the observed range and thus not unreasonable. In fact, the reported range of particulate P loss by Good et al. (2012) is relatively large (0 – 18 kg P ha⁻¹ yr⁻¹), indicating that particulate P loss is variable and site-specific, depending on crop rotations and slope, as well as other factors. Average values are thus not necessarily representative for the situation at the modelled NY farm. Further model evaluation and validation with field measurement data from different sites and various management strategies is needed to determine and, if necessary, to improve, model accuracy. This is considered important, because of the relatively large difference in predicted P erosion losses by IFSM and APEX and because P loss from agricultural soils continues to contribute to surface water eutrophication in the US (e.g. Michalak et al. 2013). ManureDNDC and DayCent do not explicitly model erosion losses, although ManureDNDC incorporates these losses into the run-off rate. At present, the DayCent model does not account for slope and erosion and is thus a poor model for P dynamics at the landscape scale.

All models predicted a relatively high amount of unaccounted N in the soil (24,483– 48,043 kg N yr⁻¹). However, long-term storage of N in soil pools is not considered realistic. The unaccounted soil N resulted from continuous over application of manure and fertilizer N on cropland, particularly on the corn fields. This N will even-

403 tually disappear from the system through leaching, erosion, run-off and/or gaseous losses. The final fate and
404 form is difficult to predict with the current model simulations. Simulated annualized soil P accumulations were
405 similar for DayCent, IFSM and APEX ranging from 9,108 to 12,524 kg P. ManureDNDC predicted a higher soil P
406 accumulation of 25,983 kg P yr⁻¹, which is consistent with the model's low simulated P in crop yields. In contrast
407 to N, long-term accumulation of soil P is expected.

408 Model predictions of soil C change were highly variable ranging from a substantial depletion in soil organic
409 carbon content of - 683,967 kg C yr⁻¹ as predicted by APEX to a substantial carbon sequestration of 629,301 kg
410 C yr⁻¹ as predicted by ManureDNDC. It should be noted, that, in this study, ManureDNDC was run for a 9 year
411 period, which is not long enough to reach steady-state in the soil carbon pool. This is confirmed by a plot of an-
412 nual soil C change per year for the complete simulation period (SI Fig. S1), which shows that annual soil C
413 change is not yet in steady-state and is in fact decreasing substantially from 1427 Mg C yr⁻¹ in the first simula-
414 tion year to 598 Mg C yr⁻¹ in the last simulation year. The ManureDNDC results therefore represent initial
415 changes in soil C content. Both IFSM and DayCent predict a negligible change in soil organic carbon content.
416 Presently, IFSM does not explicitly predict soil C change, i.e. the long term soil C change is assumed to be neg-
417 ligible. The rationale is that the farm has been following similar field practices for a relatively long period of
418 time and it is therefore assumed that the cultivated soil is in balance. This is corroborated by DayCent predic-
419 tions (SI Fig S1). DayCent was run with a 20 year spin-up period and a plot of annual soil C change per year
420 shows that a steady-state has been reached at the end of the model spin-up period (SI Fig. S1). This is not the
421 case for APEX: according APEX simulations the soil C content does not reach steady-state in the 20 year spin-up
422 period and continues to decrease during the following 14 year model simulation, resulting in a soil C decrease
423 of approximately 0.7 t C ha⁻¹ yr⁻¹ for the 14 year model simulation period (SI Fig. S1). Consistently, West and
424 Post (2002) suggested that soil C pools under enhanced crop rotation practices can take 40 to 60 years to reach
425 steady-state. This indicates that a commonly used spin-up period of 20 years (IPCC, 2006) may not be sufficient
426 to reach steady-state in the soil organic carbon pool. The predicted direction of soil C change by APEX, that is a
427 loss of soil carbon, is also noteworthy considering recent interests in adopting beneficial field management

practices to sequester atmospheric C in agricultural soil and hence, mitigate climate change (e.g. Lal, 2004). Beneficial field management practices, such as reduced tillage and enhancing crop rotation complexity, have been shown to result in soil C sequestration in long-term field trials (Lal et al. 1999; West and Post, 2002). Considering that the simulated NY farm uses minimum tillage (chisel plow) and has a relatively complex crop rotation schedule, including the cultivation of perennial crops (alfalfa), a soil C sequestration may be expected. The influence of agricultural field management practices on the soil carbon cycle is however complex and highly location-specific, as soil organic carbon contents depend on agricultural management practices, including tillage, fertilizer applications, crop residue management and crop rotation schedules, as well as the original soil C content, local soil type and climate conditions (Schmidt et al., 2011; Stockman et al. 2013). Presently, evidence on soil C sequestration potential in agricultural soils with altered management practices is conflicting. A recent long-term field experiment in Arlington, Wisconsin, showed a net loss of soil carbon of 12 t C ha^{-1} ($\sim 0.6 \text{ t C ha}^{-1} \text{ yr}^{-1}$) over a 20 year period across six different cropping-systems including several systems with beneficial management practices (no-till, enhanced crop rotation complexity, inclusion of perennial crops) (Sanford et al. 2012). Similarly, a global meta-analysis from Luo et al. (2010) indicates that cultivation for more than 5 years, on average, results in SOC loss of more than 20 t ha^{-1} in the top 60cm soil profile, with no significant differences between conventional tillage and no-till. These empirically-observed C losses, particularly from Sanford et al. (2012), are comparable with APEX predictions. However, considering the conflicting evidence on the effect of altered beneficial management practices on the soil's ability to sequester or emit carbon, it cannot be concluded yet whether APEX predictions are right or wrong. Additional long-term (>20yrs) agricultural field experiments and modelling research are needed to provide more insights on the main factors driving these changes in soil carbon pools. This is particularly relevant as soil C change can have an important impact on the total global warming potential for the field and the whole farm (see below).

3.3 Global warming impact (GWI)

Predicted whole-farm GWIs were similar for IFSM and ManureDNDC with a predicted GWI of approximately 10.8 and $9.3 \text{ Gg CO}_2\text{eq yr}^{-1}$ for IFSM and ManureDNDC, respectively (Figure 5a). This result is surprising, given

the observed differences in simulated nutrient and carbon flows by IFSM and ManureDNDC. However, in both model predictions, enteric CH₄ emissions dominate GWIs at the individual farm level with a contribution of 70% and 47% to the whole-farm GWI for IFSM and ManureDNDC, respectively. Predicted total CH₄ emissions for the barn (enteric + barn floor emissions) were very similar for IFSM and ManureDNDC, resulting in a similar predicted total global warming impact. The finding that enteric CH₄ emissions dominate whole-farm global warming potentials is consistent with results from other studies. Thoma et al. (2013) showed that enteric CH₄ emissions contribute 25% of the total C footprint of the dairy supply chain. In addition, Del Prado et al. (2013) found that enteric CH₄ and crop land N₂O were the main contributors to whole-farm GHG impacts for grassland ruminant-based farm systems in Europe, although large site- and farm-specific variations were observed. In IFSM simulations, N₂O emissions from cropland constitute an important contribution (12%) to the total GWI of the farm. In contrast, ManureDNDC predicted N₂O emissions from fields to contribute negligibly (0.01%) to total global warming potential. Nitrous oxide emissions from the barn floor are, however, a non-negligible contributor to greenhouse gas impacts (10% contribution) according to ManureDNDC. Indirect N₂O emissions contribute non-negligibly to the total, whole-farm global warming potential, with a predicted contribution of 5% and 10% for IFSM and ManureDNDC, respectively. In both model simulations, field NH₃ emissions and nitrate leaching are the dominant contributors to these indirect N₂O emissions.

The difference in predicted whole-farm global warming potentials between IFSM and ManureDNDC is attributable to the difference in predicted soil C change. ManureDNDC predicted an annual net sequestration of CO₂, resulting in a reduction in global warming potential, whereas IFSM predicted no changes in soil organic carbon pools. Total GWIs for the field are variable. IFSM, APEX and DayCent predicted a positive GWI ranging from 1.77 Gg CO₂eq. yr⁻¹ to 3.36 Gg CO₂eq. yr⁻¹, whereas ManureDNDC predicted a negative GWI of -1.36 Gg CO₂eq. yr⁻¹. These differences are attributable to differences in predicted soil C change, corroborating the above identified need for further experimental and modelling research to identify and quantify the main factors driving changes in carbon sequestration.

3.4 Implications and recommendations – individual model performance

478 Model comparison studies are often based on a comparison of model predictions with empirical data to
479 assess individual model performance and to identify which model performs best. However, technical and fi-
480 nancial constraints make it difficult to empirically determine all relevant N, P, C flows on a farm (Rotz et al.,
481 2010). Process-based models are, therefore, commonly evaluated with results from chamber experiments
482 and/or experimental data obtained from small-scale experimental “model” farms. This provides valuable in-
483 sights in model performance for individual processes, but it only allows for a partial evaluation as models are
484 evaluated only for those farm components and N, P, C flows for which measured data are available. Here, we
485 used a model cross-comparison to evaluate the performance of five process-based models in terms of N, P, C
486 flows associated with milk production. All models were set-up to represent a commercial dairy farm in NY state
487 and simulated N, P, C flows were compared using a (whole-farm) mass-balance framework. This allows us to
488 evaluate model performances for a ‘real’ commercial dairy farm, including all relevant farm components and
489 an all relevant N, P, C flows, including internal ones. The whole-farm mass-balance framework and the quantifi-
490 cation of potential global warming impacts allow us to put observed deviations in model predictions into pers-
491 pective and to prioritize areas of improvement (model-specific and overall) and thus research efforts and finan-
492 cial resources. This study can inform and complement model validation studies with empirical data.

493 In our cross-comparison, we included two whole-farm models, ManureDNDC and IFSM. ManureDNDC is an
494 extension of the DNDC (denitrification-decomposition) model, which was originally developed to simulate C
495 and N biogeochemistry in agro-ecosystems (Li et al. 2012). A specific strength of ManureDNDC is that this
496 model provides a mechanistic, biogeochemical understanding of potential differences in emissions associated
497 with different farm strategies. However, our results show that ManureDNDC predictions of soil P and crop P
498 yield, N, P, C loss with erosion, and N, P, C in milk production, are underestimated, suggesting that Ma-
499 nureDNDC performs less well for simulating processes / flows outside its core. ManureDNDC predictions of NH_3
500 volatilization and field N_2O emission are also at the extreme end of the obtained range. This is attributable to
501 model-specific differences in simulating anaerobic digestion and subsequent changes in labile C content of the
502 digestate, as discussed previously. A particular strength of IFSM is that it provides other important inputs such

as machinery use and infrastructure to determine upstream impacts. In addition, IFSM quantifies emissions associated with on-farm machinery use and enables one to quantify economic parameters, such as total production costs. Our results furthermore show that IFSM predictions generally fall within the range of the other model predictions. A current limitation of IFSM is that the model does not predict soil C change. However, considering the uncertainty regarding the factors driving soil C change, further research is needed before this process can be reliably predicted and added to the model framework. Next to the two whole-farm models, we included three component-specific models in our comparison: an animal model (CNCPS) and two field models (DayCent and APEX). The obvious limitation of using component-specific models for a whole-farm analysis is that these models simulate only one specific farm component (here, animal or field). However, since the availability of whole-farm models is currently limited, component-based models were included in our comparison to obtain simulations from multiple models. The strength of field models such as DayCent and APEX is that they can provide detailed, i.e. spatially- and temporally-explicit, accounts of N, P, and C flows at the field level. For DayCent, two areas of improvement were identified: First, DayCent does not yet simulate NH_3 volatilization from manure application on the field. For the model input, the $\text{NH}_3\text{-N}$ in manure that potentially volatilizes has to be subtracted from the total N in manure. Further development is necessary as NH_3 volatilization is the major loss pathway for N in manure (see results). Second, DayCent does not yet account for slope and erosion and is presently a poor model for P dynamics at the landscape scale. APEX predictions of N, P, C losses through erosion are substantially higher than predicted N, P, C losses through erosion as simulated by IFSM. A comparison of predicted P losses with (limited) representative field monitoring data shows that both model predictions are in the range of observed particulate P loss. The reported range is, however, relatively large ($0 - 18 \text{ kg P ha}^{-1} \text{ yr}^{-1}$). Further evaluation of both models with field measurement data covering a range of landscape conditions (particularly slope) and management practices is needed to determine model precision and to further improve model accuracy.

4. Conclusions

Overall, our results show that model predictions were comparable for most flows related to the animal, barn and manure management system, including enteric emission of CH₄ as well as NH₃ emissions from the barn. The models simulated a large range in N₂O emissions from the barn. Further model evaluation is required using empirical data of manure N₂O emissions in free stall barns as a function of manure handling strategies. Predicted field emissions of N₂O and NH₃ as well as N and P losses to the hydrosphere and soil C change were highly variable across models. This indicates there is a need to further our understanding of soil and crop nutrient flows and that measurement data on nutrient emissions and carbon flows are particularly needed for the field. Priority research areas for process-model evaluation and improvement include soil P (erosion) loss, soil C change and anaerobic digestion. For soil P loss, field measurement data of soil P loss covering a range of landscape conditions (particularly slope) and management practices is needed for model evaluation and to further improve model accuracy. This is of importance as P loss from agricultural soils continues to contribute to surface water eutrophication in the US (e.g. Michalak et al. 2013). For soil C change, long-term (>20 yrs) agricultural field experiments are required to study the impact of beneficial management practices on soil organic carbon pools. This is of importance as *i*) our results show that model predicted deviations in soil C change have a large impact on whole-farm and field global warming carbon impacts and *ii*) carbon sequestration in agricultural soils through altered (beneficial) management practices has been advocated as a measure to mitigate climate change (e.g. Lal, 2004). In addition, there is a need to further understand how the anaerobic digester influences manure composition and subsequent emissions of N₂O and NH₃ after application of the digestate to the field. Empirical data on manure composition before and after anaerobic digestion are essential for model evaluation. This is a priority research area considering the wide interest in future, large-scale implementation of anaerobic digesters to reduce methane emissions from livestock waste (e.g., EPA, 2011, Defra, 2011).

This model comparison study has implications for whole-farm nutrient management studies and farm-gate Life Cycle Assessment (LCA) studies that aim to evaluate nutrient efficiency optimization and/or GHG mitigation strategies of dairy production systems. Our results suggest that the animal, barn and manure management components are relatively well understood and that process-models can be used to reliably quantify GHG and

552 nutrient-based emissions for these farm components. Estimates of field related emissions are more variable
553 and a detailed comparison with empirical data is required to further enhance and test model accuracy for field-
554 based emissions and to select the most appropriate models to predict emissions for the field.

555 Our study furthermore highlights the importance of using whole farm models to account for the interde-
556 pendence between emission flows in the different farm compartments. For LCA and carbon foot printing stu-
557 dies, it is therefore recommended to use a whole-farm process-based model to quantify farm-component spe-
558 cific emissions. Based on our model comparison, we suggest utilizing IFSM as a whole farm model baseline, at
559 this stage, as IFSM can simulate all relevant flows and IFSM predictions generally fall within the range of the
560 other model predictions. In addition, IFSM provides other important inputs essential for LCA studies such as
561 machinery use and infrastructure to determine upstream impacts. IFSM also allows a quantification of emis-
562 sions associated with on-farm machinery use and enables one to quantify economic parameters, such as total
563 productions costs. The other models can be used to support and/or check IFSM predictions, but only if the
564 above mentioned individual model limitations are taken into consideration.

565 Finally, it should be reiterated here that our model comparison study is based on model simulations for a
566 single commercial dairy farm in NY State. The predicted flows are therefore representative for the considered
567 farm characteristics (including farm size, herd type, crops grown, manure management system), field manage-
568 ment practices, and location-specific environmental conditions (soil characteristics and weather). Predicted N,
569 P and C flows are therefore likely different when the models are run for a different farm, at a different location.
570 We do however expect that our conclusions regarding individual model performances and our overall recom-
571 mendations will qualitatively hold.

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Figure 1. Whole-farm mass-balance framework for considered nutrient and carbon flows. All nutrient flows in kg N yr^{-1} or kg P yr^{-1} and all carbon flows in kg C yr^{-1} . Black arrows represent internal nutrient flows, blue arrows represent nutrient and/or carbon inflows to the farm whereas orange arrows represent nutrient and/or carbon losses from the farm. To quantify global warming impacts, next to soil C change, emissions of 2 greenhouse gases were considered, N_2O and CH_4 , which are indicated in green letters.

Figure 2. Nitrogen mass-balances: whole-farm mass-balances for IFSM and ManureDNDC and field mass-balances for APEX and DayCent. The empirically-derived (import-export) balance is added for comparison. Underlined flows were model inputs, all other flows were predicted by the models. For DayCent and APEX, model simulations were performed based on the manure application rate as predicted by IFSM as further described in the methods. *IFSM contains an animal sub-model that predicts all feed and purchased feed supplements needed to meet the protein and energy requirements of all animals. **Note that DayCent predicts NH_3 volatilization from harvested and senesced biomass N and does not predict NH_3 volatilization from manure application. For DayCent simulations the amount of $\text{NH}_3\text{-N}$ in manure, as estimated by IFSM, was therefore subtracted before manure field application. This results in a lower amount of manure N applied in DayCent ($155,320 \text{ kg N yr}^{-1}$) compared to the other models, incl. APEX ($198,949 \text{ kg N yr}^{-1}$). n.a. = not available, that is not simulated by the model.

Figure 3. Phosphorus mass-balances: whole-farm mass-balances for IFSM and ManureDNDC and field mass-balances for APEX and DayCent. The empirically-derived (import-export) balance is added for comparison. Underlined flows were model inputs, all other flows were predicted by the models. For DayCent and APEX, model simulations were performed based on the manure application rate as predicted by IFSM as further described in the methods. *IFSM contains an animal sub-model that predicts all feed and purchased feed supplements needed to meet animal requirements including phosphorus. n.a. = not available, that is not simulated by the model.

Figure 4. Carbon mass-balances: whole-farm mass-balances for IFSM and ManureDNDC and field mass-balances for APEX and DayCent. Underlined data were model inputs, all other data are predicted by the models. For DayCent and APEX, model simulations were performed based on the manure application rate as predicted by IFSM as further described in the methods. *IFSM contains an animal sub-model that predicts all feed and purchased feed supplements needed to meet the protein and energy requirements of all animals. n.a. = not available, that is not simulated by the model. **Note that predicted CO_2 and CH_4 emissions from manure are not directly comparable for IFSM and ManureDNDC. ManureDNDC predicts CO_2 and CH_4 emissions from the lagoon and the composition of biogas (in terms of C). IFSM emissions are those leaving the farm, thus the CO_2 emission includes that from biogas combusted in the turbines driving the electric generators or in the boiler heating water.

Figure 5. Predicted global warming potentials (GWP) for the whole-farm (a) and the field (b) (in $\text{Gg CO}_2 \text{ eq. yr}^{-1}$).

Farm components – Mass balance compartments

Animal: total herd; Barn: animal housing facility; Manure: storage system, i.e. digester + lagoon; Soil: tillable crop acres; Crops: alfalfa, corn, winter wheat, grass; Feed: all animal feed

Internal flows [kg N yr⁻¹, kg P yr⁻¹, kg C yr⁻¹]

1. Feed; 2. Manure (urine + dung) excreted; 3. Collected manure; 4. Bedding material – manure solids; 5. Manure applied; 6. Crop nutrient uptake from soil; 7. Crop residue; 8. Harvested crop yield (excl. cash crops)

Storage / remaining [kg N yr⁻¹, kg P yr⁻¹, kg C yr⁻¹]

[A] Remaining in barn, i.e. on floor, in gutter; [B] Remaining in digester and lagoon; [C] Nutrient accumulation in soil; [D] Feed stored

a. Empirical N balance

b. IFSM N balance

c. ManureDNDNC N balance

d. APEX field N balance

e. DayCent field N balance

a. Empirical P balance

b. IFSM P balance

c. ManureDND C P balance

d. APEX field P balance

e. DayCent field P balance

5a. Whole-farm

5b. Field