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Challenges and opportunities to capture dietary effects in on-farm greenhouse gas emissions models of ruminant systems

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Short title: Dairy diet characteristics and on-farm greenhouse gas emission models

Abstract

This paper reviews existing on-farm GHG accounting models for dairy cattle systems and their ability to capture the effect of dietary strategies in GHG abatement. The focus is on methane (CH_4) emissions from enteric and manure (animal excreta) sources and nitrous oxide (N_2O) emissions from animal excreta. We identified three generic modelling approaches, based on the degree to which models capture diet-related characteristics: from 'none' (Type 1) to 'some' by combining key diet parameters with emission factors (EF) (Type 2) to 'many' by using process-based modelling (Type 3). Most of the selected on-farm GHG models have adopted a Type 2 approach, but a few hybrid Type 2 / Type 3 approaches have been developed recently that combine empirical modelling (through the use of CH_4 and/or N_2O emission factors; EF) and process-based modelling (mostly through rumen and whole tract fermentation and digestion). Empirical models comprising key dietary inputs (i.e., dry matter intake and organic matter digestibility) can predict CH_4 and N_2O emissions with reasonable accuracy. However, the impact of GHG mitigation strategies often needs to be assessed in a more integrated way, and Type 1 and Type 2 models frequently lack the biological foundation to do this. Only Type 3 models represent underlying mechanisms such as ruminal and total-tract digestive processes and excreta composition that can capture dietary effects on GHG emissions in a more biological manner. Overall, the better a model can simulate rumen function, the greater the opportunity to include diet characteristics in addition to commonly used variables, and thus the greater the opportunity to capture dietary mitigation strategies. The value of capturing the effect of additional animal feed characteristics on the prediction of on-farm GHG emissions needs to be carefully

balanced against gains in accuracy, the need for additional input and activity data, and the variability encountered on-farm.

Keywords: Dairy farm system, Diet, Feeding management, Effluent, Methane, Nitrous oxide.

1. Introduction

In recent years, there has been an increasing focus on evaluating the environmental effects of livestock production systems, including their impact on greenhouse gas (GHG) emissions. Although debate remains on the precise contribution of ruminant livestock to anthropogenic methane (CH_4) (Hristov *et al*., 2018), the role of livestock agriculture as a main contributor to GHG emissions and climate change is undisputed. Climate change and its consequences are currently recognised as one of the major environmental challenges, and the need for GHG mitigation to meet local expectations and international environmental obligations has been globally recognised (Smith *et al*., 2007). Therefore, it becomes increasingly important to have an enhanced ability to predict on-farm GHG emissions from livestock and assess methods and efficacy of practices to reduce or offset them.

In livestock agriculture, interactions and variability of critical environmental and managerial drivers of GHG emissions contribute to the complexity of extrapolating observed GHG data to a broader range of conditions and scales. Simulation models of on-farm greenhouse gas (GHG) emissions have an important role to play in helping us understand the potential impact of GHG mitigation strategies on farm dynamics, and in using results from experimental measurements of GHG emissions to assess wider implications and potential trade-offs for the system. Models also enable extrapolation of GHG emissions from smaller (i.e., emissions from a site, plot, field, a manure storage facility or from a cow) to larger scales (farm, catchment, region or country) (Schils *et al.*, 2012). In addition to scale, models can also vary depending on the GHG of interest, with some simulating a single GHG (Blaxter and

Clapperton, 1965; Wilkerson *et al.*, 1995; Benchaar *et al.*, 2001), while other models include all major agricultural GHG (Wheeler *et al.*, 2008; Hillier *et al.*, 2011).

Given the broad range of GHG accounting tools, the complexity of the issue at hand and the increasing need for accounting of on-farm GHG emissions to meet national or global obligations, there is uncertainty amongst agricultural stakeholders as to which tools (calculators, models, modules) are most appropriate to predict GHG emissions from ruminant systems. The amount of GHG produced within a production system needs to be quantified accurately to allow for alternatives to be explored and emissions to be mitigated (Ellis *et al.*, 2010; Benaouda *et al.*, 2019). In addition to the inherent temporal and spatial variability in emissions, the relative advantages and disadvantages of these tools remain to be fully assessed, especially in light of the difficulty in comparing results obtained from different accounting tools, as these vary in conceptual approaches, reporting units and scope.

Feed management decisions are essential for ruminant production systems, as they impact directly on substrate availability for enteric microbial fermentation and digestion, nutritive value, and ruminant excreta composition. In turn, these processes have a strong influence on the amount and profile of agricultural GHG emissions (Henderson *et al*., 2015). Major sources of GHG emissions from livestock agriculture include methane (CH_4) emissions from enteric fermentation and stored manure, and nitrous oxide (N_2O) emissions from animal excreta. Accordingly, there is an increasing interest in the use of nutrition and feeding management strategies to reduce GHG emissions. A range of nutritional and feeding management options for CH_4 abatement (Beauchemin *et al.*, 2008; Martin *et al*., 2010; Caro *et al.*, 2016; Pellerin *et al.*, 2017) and N_2O abatement (de Klein and Eckard, 2008; Monaghan and

de Klein, 2014) have been described. Examples of nutrition strategies that have shown promising results in mitigating GHG emissions include increasing grain levels (i.e., greater concentration of degradable starch and soluble carbohydrates in the diet), inclusion of lipids and dietary tannins, reducing dietary crude protein, improving feed digestibility and altering the stage of maturity of harvested forages.

In 2017, a three-year project commenced to bring together the current knowledge on the effect of feed and dietary management on GHG emissions: Capturing the Effects of Diet on Emissions from Ruminant Systems (CEDERS; https://www.eragas.eu/en/eragas/Research-projects/CEDERS-1.htm). The main goal of the project was to examine dietary effects on on-farm GHG emissions and their trade-offs, both at the farm and national scales, with the overall aim of supporting GHG mitigation research and aligning national agricultural GHG inventory research across a consortium of ten countries (Chile, Denmark, Finland, France, Germany, Ireland, Netherlands, New Zealand, Sweden and United Kingdom). Our review is part of this project with the specific objectives to a) identify the most common on-farm GHG accounting tools used by the participant countries, and once identified, b) explore the livestock GHG accounting approach used by these tools, and c) explore the potential benefits of adding diet characteristics to on-farm GHG accounting tools for dairy systems. The focus is on CH_4 emissions from enteric fermentation and manure (animal excreta) and N_2O emissions from animal excreta as on-farm GHG sources.

2. Modelling GHG emissions from ruminant enterprises

Methane and N_2O are colourless and odourless GHG that are 28 and 265 times more potent (100-year horizon) than CO_2 at warming the earth (Myhre *et al.*, 2013).

Enteric and manure CH_4 emissions from ruminants, and N_2O emissions from animal excreta are the main GHG from livestock agriculture. The contribution of CO_2 emissions from energy sources and input use are frequently added to GHG budgets, often using a life cycle assessment (LCA) approach. Many mathematical models have been developed to predict these major on-farm GHG.

With a focus on the two main GHG from animal livestock systems (CH_4 and N_2O), different types of models have been developed to predict emissions of these gases. These models vary in the level of detail they capture and range from relatively simple empirical (or statistical) models to more detailed empirical and process-based mechanistic models (herein, mathematical representations of the several underlying processes that characterise the function and integration of biology leading to GHG emissions). The ability to assess the impact of dietary mitigation strategies relies on accurate estimations of enteric and manure CH_4 emissions and N_2O emissions. Estimates of enteric CH_4 emissions are often based on dry matter intake (DMI) and/or the chemical composition or other characteristics of the diet (e.g., organic matter digestibility and fibre concentration), and/or certain characteristics of the animal, such as body weight (BW) or animal product (milk or meat) (Wilkerson *et al.*, 1995). Estimates of N_2O emissions are often based on animal excreta, manure storage and processing, nitrogen (N) fertiliser and soil conditions that favour denitrification (Brown *et al.*, 2001; de Klein and Ledgard, 2005).

Although such equations and predictors provide an estimate of emissions from the animal and animal excreta (CH_4 and N_2O emissions) and from soil conditions (N_2O emissions), these equations are sometimes used in isolation. The variation due to diet types, feeding management and source (e.g., imported vs. on-farm feed) and

176 the extent to which polluting end points are affected (e.g., N in freshwater bodies),
177 are harder to capture, and as a consequence, these equations can still be poor
178 predictors of GHG emissions at a specific farm scale. At the dairy farm scale, a
179 greater complexity with integrated components such as livestock, manure
180 management, housing conditions (barn or on pasture), soil management, and
181 pasture and fodder crop production need to be incorporated in the modelling (Ellis *et*
182 *al.*, 2010).

183 ## 3. Models of on-farm GHG emissions

184 In addition to models used for GHG inventories (e.g., Ministry for Primary Industries,
185 2019) and those used for carbon cycle assessments (e.g., Cowie *et al.*, 2012), Denef
186 *et al*. (2012) classified GHG tools into four major categories: calculators, protocols,
187 guidelines and models. The focus of this review is on on-farm calculators and farm-
188 scale models (herein *on-farm GHG models*) that have been either developed to aid
189 in the representation of enteric fermentation (the prevalent source of GHG from
190 ruminant systems), or that aim to quantify GHG emissions from ruminants (or
191 improve prediction capacity), under varying animal nutrition conditions.

192 To date, a large number of on-farm GHG models have been developed for use by
193 farmers, farm consultants, environmental authorities and the scientific community.
194 On-farm GHG models can help with i) estimating total emissions for accounting
195 purposes, raising awareness, ii) identifying, developing and encouraging adoption of
196 mitigation strategies, iii) identifying knowledge gaps, and creating and exploring
197 current and alternative scenarios, and iv) scaling-up information, and making future
198 projections and policy development (Smith *et al.*, 2007; Colomb *et al.*, 2012; Milne *et*
199 *al.*, 2013).

On-farm GHG models offer a broad diversity of scope (i.e., from single GHG to integral assessment of all three major GHG), modelling approach adopted (i.e., from simple empirical approaches to more complex dynamic or process-based models), scale (i.e., from the rumen, soil plot and manure scale to global scale) and emissions source (i.e., horticulture, grazing and livestock, grasslands, orchards, forestry, and other land uses) (Hall *et al*., 2010; Schils *et al*., 2012). Although models tend to be characterised as being empirical or mechanistic, often both approaches are followed for different components within a single model. In general, farm-scale models tend to follow hybrid or empirical approaches at wider scopes and at various scales to integrate soil, crop and livestock components into a farm framework (Schils *et al.*, 2012).

The degree to which diet ingredients and diet chemical composition are captured in on-farm GHG models varies considerably. The first step at the animal level of most on-farm models is to estimate daily DMI per animal, derived from estimated animal energy requirements (often based on BW, maintenance needs, tissue growth, milk production, pregnancy, and activity) divided by the energy concentration of the feed. The gross energy (GE; in megajoules MJ) concentration of a feed can be calculated based on crude protein (CP), ether extract (EE), neutral detergent fibre (NDF) and non-fibre carbohydrate (NFC) concentrations. The major component of metabolisable energy (ME) or net energy (NE) of a feed is digestible energy (DE). The DE value of a feed can be estimated from organic matter digestibility (OMD), or from feed chemical composition (from similar components as used for calculation of GE) and corresponding digestibility coefficients published in feed tables for individual ingredients (Beyer *et al*., 2003; Blok and Spek, 2016; Rinne *et al.*, 2017). Feed DE can also be estimated using prediction equations (NRC, 2001) or be based on a

225 combination of chemical composition data and prediction equations (Fox *et al.*,
226 2004). These DE or OMD values are often used to calculate total faecal OM output
227 or volatile solids (VS), which are the source of manure CH_4 emissions. However,
228 some more advanced models predict DE, OMD, VS and N digestibility (ND)
229 mechanistically (Illius and Gordon, 1991; Bannink *et al.,* 2018, 2020).

230 The second step of the animal level model comprises the calculation of a CH_4
231 conversion factor (MCF or Y_m), which can involve a) multiplying DMI or GE intake
232 (GEI) with a fixed conversion factor [e.g., MCF (% of GE) = 6.5 ± 1.0% of GEI (IPCC,
233 2006)], b) the use of a generic equation, that might include dietary ingredients (e.g.,
234 forage and concentrate), chemical composition parameters (e.g., EE, NDF, starch)
235 and digestibility parameters (e.g., OMD) (Nielsen *et al.*, 2013; Jaurena *et al*., 2015;
236 Eugène *et al.*, 2019), or c) the use of a dynamic and mechanistic model with
237 representation of rumen fermentation and gastrointestinal digestion (Bannink *et al.*,
238 2011; Beukes *et al.*, 2011; Huhtanen *et al.*, 2015). Input parameters for these
239 dynamic, mechanistic models include DMI, diet chemical composition and ruminal
240 and total tract digestive parameters (Table 1). In these models, rumen H_2 formation
241 is derived from fermented amounts of substrate and associated volatile fatty acid
242 (VFA) stoichiometry (e.g., Bannink *et al.*, 2011; Huhtanen *et al.*, 2015).

243 The third and final step in capturing dietary effects in on-farm GHG models is an
244 estimation of CH_4 and N_2O emissions from manure storage, land application of
245 manure and direct deposition of faeces and urine by grazing animals. Both CH_4 and
246 N_2O emissions from manures are not only influenced by diet characteristics but also
247 by biotic and abiotic factors such as manure storage, soil and climatic conditions.
248 Here we focus on the influence of diet. Manure CH_4 emissions are strongly linked to

249 the VS content of the manure and as mentioned above this is often estimated from
250 DE or OMD values. Nitrous oxide emissions are calculated from the amount of N
251 excreted as faeces and urine multiplied by an emission factor (IPCC, 2006). Nitrogen
252 excretion estimates require information on DMI per animal and CP or N
253 concentration of the diet (IPCC, 2006) (Figure 1), where the N concentration of the
254 diet also influences partitioning of excreta N into faeces and urine (IPCC, 2019).
255 Excretion estimates can be refined further by accounting for improved estimates of
256 apparent faecal ND. Nitrous oxide emission factors will differ according to the
257 method of manure management and, for excreta, the livestock type (e.g., cattle vs.
258 sheep) and form of excreta (faeces vs. urine) (IPCC, 2006).

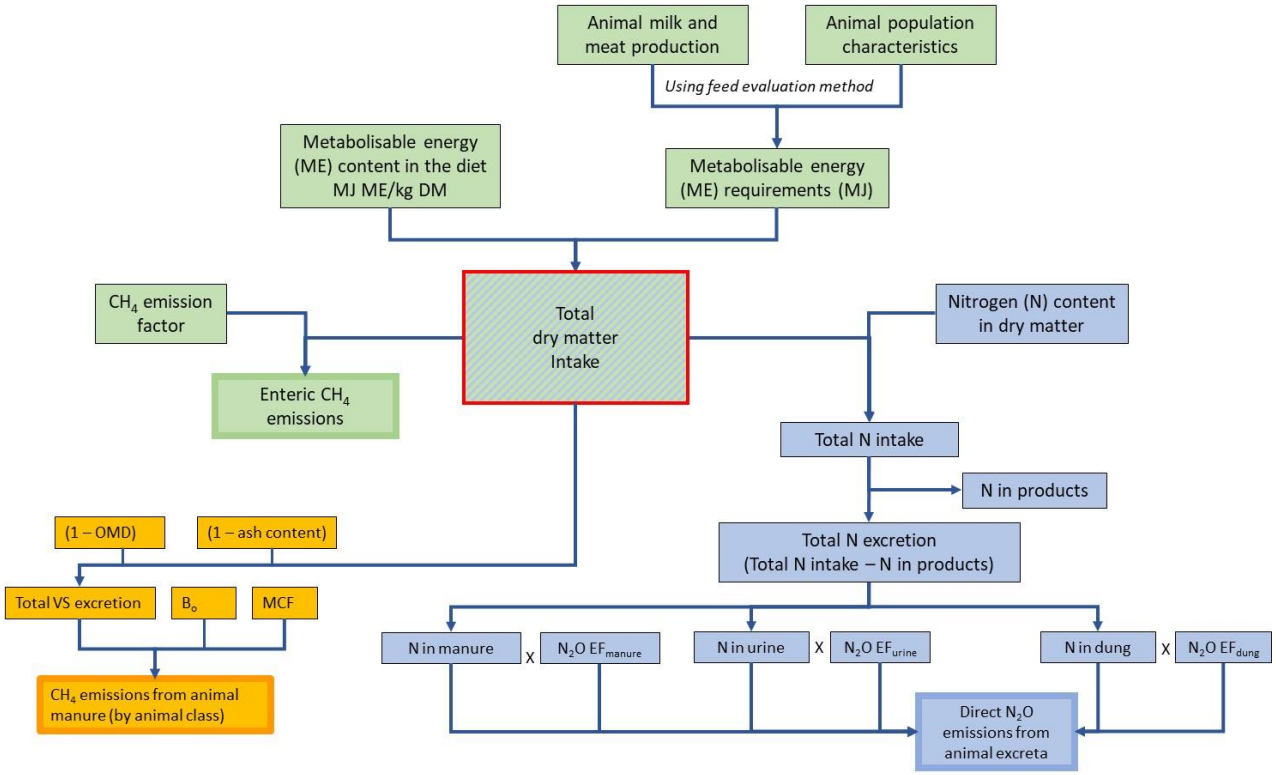
259 ## 4. On-farm GHG model approaches to capture dietary effects on GHG
260 ## emissions from livestock systems

261 In most ruminant systems, CH_4 is the predominant source of GHG emissions, with
262 the diet having a major impact on enteric CH_4 from fermentation of feed in the
263 rumen; the latter is the prevailing GHG source. For the two most important GHG
264 (CH_4 and N_2O), there are three generic approaches that on-farm models use to
265 estimate the effect of dietary characteristics on GHG emissions from livestock
266 systems. The three approaches (hereafter *Types*) differ in the level and units the
267 model is attempting to predict and quantify, and the degree at which diet-related
268 details are represented, often associated with the number of variables and modelling
269 approach chosen. The three approaches we identified are:

270 - A *Type 1* approach has a very low level of detail and uses a CH_4 emission factor
271 (EF) per animal and an N_2O EF per unit of animal excreta, similar to a Tier 1 level
272 at a national scale (IPCC, 2006).

- A *Type 2* approach has an intermediate level of detail (Figure 1). It estimates the energy requirements of the animal (often in terms of ME or NE) based on milk, meat and fibre production, and animal characteristics. These requirements are then used to estimate feed DMI; enteric CH_4 emissions are then estimated using a CH_4 EF (g CH_4 kg^{-1} DMI).
- A *Type* 3 approach has a higher level of detail that often involves process-based modelling, taking into account DMI, diet chemical composition and nutrient supply, along with feed degradation and fermentation characteristics to predict (rather than assume) CH_4 EF according to a mechanistic, dynamic representation.

Type 1 models that use a default EF per animal or per unit of excreta N are not commonly used for on-farm GHG accounting or LCA, and generally only serve at a national level for inventory purposes. However, some on-farm GHG accounting models use country-, region- or farm-specific EF and apply these to the number of animals (e.g., kg CH_4 $animal^{-1}$ $year^{-1}$) or the amount of excreta N (e.g., kg N_2O-N kg^{-1} N excreted) (*diversified* Type 1 models; herein Type 1+ models). The EF for these Type 1+ models can be derived from experimental data (e.g., van der Weerden *et al.*, 2011; Chadwick *et al.*, 2018) or from detailed process-based modelling that could also provide look-up tables of EF (e.g., based on farm system, animal type or region) for such Type 1+ models. Type 1 models that use IPCC default values cannot capture dietary effects as CH_4 and N excreta EF are provided for an *average* animal. However, Type 1+ models could capture dietary effects if experimental data or results from process-based models deliver different EF estimates for an animal (or per unit of N excreta) consuming different diets.



297

298 **Figure 1.** Schematic overview of a generic Type 2 approach for estimating methane (CH_4) and nitrous
299 oxide (N_2O) emissions from livestock production systems (modified from de Klein *et al*., 2019). Green
300 boxes refer to enteric CH_4, orange boxes to manure CH_4, and blue boxes to N_2O. ME = metabolisable
301 energy; MJ = mega joules; OMD = organic matter digestibility; VS = volatile solids; B_0 = maximum
302 CH_4 producing capacity of manure; MCF = CH_4 conversion factor; EF = emission factor. The
303 efficiency of use of feed energy and protein modulate these fluxes.

304

305 For Type 2 models, a number of alternative approaches have been followed. These
306 include either a) models that calculate energy requirements to estimate DMI with
307 fixed EF and N excreta values, with or without different EF values for different stock
308 classes (e.g., Wheeler *et al.*, 2008), b) models that use prediction equations for
309 enteric CH_4 emissions or for EF estimates based on feeding level, dietary proportion
310 of concentrate and OM digestibility (OMD) from a large literature database (e.g.,

311 Eugène *et al.*, 2019), or c) a purely experimentally-driven (empirical) estimate of EF
312 rather than a meta-analysis (e.g., Hellwing *et al.*, 2016).

313 For models using Type 2a approaches, the opportunities to capture GHG abatement
314 from ruminants using diet characteristics are limited. The use of sole indicators of
315 diets or diet components feeding values such as ME, often calculated from chemical
316 composition and OMD (irrespective of feeding level), limits the possibilities of GHG
317 mitigation via nutritional strategies (Waghorn, 2007; Niu *et al.*, 2018). This approach
318 tends to use animal-, rather than feed-driven EF, and appears less accurate in
319 accounting for changes in diet and diet characteristics other than by changes in
320 feeding value. A more detailed alternative to this approach is the use of specific
321 dietary ingredient EF (i.e., different EF for concentrates, supplements and fresh
322 forages). Following this approach, emissions from enteric fermentation are
323 calculated using different EF (g CH_4 kg^{-1} DMI) values for concentrates, maize silage
324 and grass products (Schils *et al.*, 2006), most likely obtained from respiration
325 chambers. Type 2b models have a few more opportunities to capture GHG
326 abatement using diet characteristics. However, these are limited to the predictor
327 variables included in the empirical enteric CH_4 equation (feeding level, OMD and
328 dietary proportion of concentrate) and the characterisation of non-digestible OM (CP,
329 NDF, starch, C/N ratio) and N excretion (urinary and faecal), and its effect on manure
330 EF (INRA, 2018; Eugène *et al.*, 2019). Finally, models that follow Type 2c
331 approaches have greater opportunities to explore GHG abatement using diet
332 characteristics by using different EF based on experimental studies. For example,
333 some experiments have shown that an increased concentration of starch and fat in
334 the diet resulted in a significantly lower CH_4 conversion factor (MCF, % of GEI)
335 (Hellwing *et al.*, 2016; Niu *et al.*, 2018; Sauvant *et al.*, 2018).

Alternatively, process-based models could be used to provide diet-specific EF. For example, Bannink *et al.* (2020) recently derived lookup tables for specific EF for feeds and dietary ingredients for a range of diet classes (classified according to the proportion of maize silage in forage DM) and estimating DMI from process-based modelling. In this way, the essence of variation predicted by a process-based modelling approach (Type 3) was introduced by differentiation of EF values and correction for DMI and diet class in an otherwise typical Type 2a approach.

In all Type 2 models, estimates of DMI, along with the N concentration of the feed, are used to estimate animal N intake, which provides the basis for estimating N excretion in urine, faeces and manure effluent. Nitrous oxide emissions from these sources are then estimated using source-specific EF (e.g., Wheeler *et al*., 2008). Furthermore, to explore GHG abatement, the partition between faecal and urinary N fluxes derived from N intake can be estimated (INRA, 2018) along with CH_4 emissions for some mitigating strategies (e.g., for forage diets by Sauvant *et al*., 2014 in the INRA Method; for various diets by deriving an ND correction factor by Bannink *et al*., 2018 in DairyWise).

A Type 3 approach considers the effect of feed intake, feed chemical composition, ruminal degradation characteristics and end-products of fermentation, as well as rumen fermentation conditions and physical inflows and outflows of nutrients, to estimate enteric CH_4 emissions (e.g., Bannink *et al.*, 2011; Beukes *et al*., 2011; Huhtanen *et al.*, 2015). This is often achieved using process-based (mechanistic) models that focus on detailed biological and physical processes with explicit mechanisms being represented, in contrast to the empirical approaches with Type 2

359 models which are typically simpler, and the mechanisms are made implicit to the
360 model.

361 Nitrous oxide emissions are largely estimated as for Type 2, but feed characteristics
362 are used to estimate faecal N digestibility and N returned to the different soil N pools
363 and processes (Bannink *et al.*, 2018; INRA, 2018). In this way, Type 3 approaches
364 allow for dietary ingredients, feed composition and digestion kinetics to be
365 considered not only for CH_4 but also for N excretion and associated N_2O accounting
366 and mitigation.

367 5. Selected on-farm GHG models

368 We have selected a number of (*on-farm and animal*) models from CEDERS
369 participant countries, mostly based on degree of adoption and use, and on published
370 literature. Information on these models was either publicly available or provided by
371 experienced users. A brief description of the selected models is provided as
372 Supplementary Material. The source of the model, the inclusion of diet
373 characteristics and digestion kinetics in calculating enteric CH_4, are described in
374 Table 1. Similarly, the inclusion of diet characteristics in calculating manure-derived
375 CH_4 and N_2O from N excreta, are presented in Table 2.

376 5.1 Brief summary of the models

377 Most of the selected on-farm GHG models have adopted a Type 2 approach,
378 generally using CH_4 and N_2O emission factors (EF) or a CH_4 conversion factor
379 (MCF). Recently, a few hybrid Type 2 / Type 3 approaches have been developed
380 that combine empirical modelling (through the use of CH_4 or N_2O EF) and process-
381 based modelling, mostly of rumen and whole tract fermentation and digestion.

382 Obtaining an accurate estimation of DMI is an essential first step to obtain accurate
383 GHG predictions, because this variable is such an overriding factor in enteric CH_4
384 emissions. It also leads to predictions of OM excretion (i.e., VS), manure CH_4
385 emissions, and to predictions of N excretion, in turn a major predictor of N_2O
386 emissions. Estimates of DMI in these models are often obtained from either feed
387 tables or nutrition models (energy based or protein-plus-energy based) (e.g.,
388 Scandinavian feed units in FarmGHG; the NE_L system in GAS-EM; CSIRO (2007) in
389 OverseerFM) (Type 2 approach) or as an outcome of more sophisticated models. In
390 experimental settings, measuring feed on offer vs feed refused (housing systems),
391 inference from animal performance (housing and grazing systems), and the use of
392 markers and estimates from herbage disappearance (grazing systems), are
393 commonly used to obtain estimates of DMI. In turn, the information collected in these
394 settings provides a feedback loop to keep feed tables, nutrition models and ruminant
395 models relevant and updated.

396 A second step in this process is the attainment of adequate EF (i.e., CH_4 per unit of
397 DMI and per unit of faeces at grazing, CH_4 and N_2O per unit of animal excreta).
398 Emission factors are often obtained from either literature surveys, databases of
399 experimental data, or based on predictions of process-based models that are able to
400 be explanatory and consider further detail. The choice will depend on country- or
401 region-specific data availability and the possibility of adapting and validating the later
402 models to country- or region-specific conditions.

403 A subtle distinction can be made between empirical GHG prediction models that
404 potentially represent the most relevant results obtained from experimental work, and
405 mechanistic models that attempt to grasp the underlying mechanisms and

406 processes. In ruminants, enteric CH_4 is primarily produced in the rumen (87% of total
407 enteric CH_4 production) and to a lesser extent in the large intestine (the remaining
408 13%) (Murray *et al*., 1976; Torrent and Johnson, 1994; discussed in Ellis *et al*.,
409 2008). The closer the models are at interpreting and simulating rumen function
410 (ruminal degradation characteristics and end-products of fermentation), the greater
411 the opportunity to capture diet characteristics beyond the sole variables OM or DM
412 intake, and to capture dietary mitigation alternatives.

413

414 **Table 1**. Feed characteristics, digestion processes of enteric methane (CH_4) calculations in selected on-farm models.

Model (main source), country, and model type	Feed characteristics and processes used for enteric CH_4 calculations		
	Feed components and feed characteristics	Digestion kinetics	Enteric CH_4 calculation
Karoline (Danfær *et al.*, 2006) – Denmark / Sweden. Type 3 model.	Forage (for) pdNDF, concentrate (con) pdNDF, for iNDF, con iNDF, starch, lactic acid, NH_3-N, free aa, peptides, soluble CP, insoluble CP, pdCP, for EE, con EE, rest fraction [DM – (ash + NDF + starch + lactic acid + VFA + CP + EE)] (contains WSC, pectins, organic acids, alcohols). VFA for silages.	Feed-specific digestion rates (kd) for pdNDF, insoluble CP and starch. Digestion rate (Kd) of pdNDF adjusted for dietary NFC and feeding level.	Rumen H_2 based on VFA stoichiometry from fermented feed, adjusted for feeding level. H_2 pool adjusted for microbial mass and BH. Includes CH_4 formation in hind gut.
FarmGHG (Olesen *et al.*, 2006) – Denmark. Type 2 model.	CF, NFE, CP, and fat daily intake (kg d^{-1}).		Empirical equation (Kirchgessner *et al.*, 1995).
Valio Carbo® Farm calculator – Finland. Type 2 model.	DMI, OMI, GE, ME, DM, ash, OMD, FOM, CP, EPD, EE, NDF, iNDF, AAT, feed-AAT; PBV, NFC, NFC/CHO lactic acid, VFA, ammonia (g kg^{-1} N), Ca, P, Na, Mg, K, S, Cl, Fe, Cu, Zn, Mn, I, Co, Mo, Se, WSC, starch, iNDF, CF, NFE.	Digestibility of CP, EE, CF, NFE, OM.	Empirical equations (Ramin and Huhtanen, 2013).
FarmSim (Graux *et al*., 2011) – France. Type 2 model.	For and con NDF, digestibility. Grazing: adjusted for dietary NE intake and animal needs.		IPCC Tier 1 (274 and 279 g CH_4 d^{-1} for European and Dutch dairy cows, respectively) and Tier 2 (MCF = 6% of dietary GEI) (IPCC, 1996).
INRA Method (Eugène *et al*., 2019) – France. Type 2/3 model.	Not a farm-scale model, but used to progress from Tier 2 to Tier 3 at a national scale. Energetic requirements: GE, DE, NEL. Feed characteristics: DM, OM, CP, NDF, OMD, PC, N balance in the rumen.	Digestibility of OM, NDF, CP, starch, N. Digestive interactions driven by feeding level, DMI and BW. Also includes digestion rates (kd), N and energy use efficiencies.	Empirical equations (Sauvant and Nozière, 2016). Mitigation options (Sauvant *et al*., 2018).
GAS-EM (Haenel *et al*., 2020) – Germany. Type 2 model.	GE, DE, NEL, DM, OM, ash, CP (and/or N); OMD, CF, NFE, and fat. No differentiation by seasons and regions.		Empirical equation (Kirchgessner *et al.*, 1994).
The GHG model (O'Brien *et al.*, 2010) – Ireland. Type 2 model.	Dairy cows on conserved forage: proportion of forage in the diet and total DMI. Dairy cows on fresh grass: 0.065 × GEI (IPCC, 2006).		Empirical equations (Mills *et al.*, 2003; IPCC, 2006).
DairyWise (Schils *et al.*, 2007) – Netherlands. Type 2/3 model.	Different EF for con, maize silage and grass products (20, 22 and 27 g CH_4 kg^{-1} DMI, respectively). Updated (Bannink *et al*., 2020) with EF for different feeds (con ingredients, for qualities and diet types; the latter based on % maize silage in dietary for) derived from Dairy Tier 3 simulation.		CH_4 EF × animal intake (Schils *et al.*, 2006). Updated and corrected CH_4 EF values (Bannink *et al*., 2020).
Dairy Tier 3 (Dijkstra *et al*., 1992; Bannink *et al*., 2011) – Netherlands. Type 3 model.	DMI, aNDFom, starch, SC, CP, non-ammonia CP, crude fat, ash, organic acids (for silages, lactic acid and VFA), and non-allocated OM, now allocated to sugars, starch and aNDFom depending on the ingredient type.	*In situ* degradation of aNDFom, starch and CP for each diet ingredient [washable fraction (W), potentially degradable (D), and	Rumen H_2 based on VFA stoichiometry from fermented substrate (SC, starch, HC, Ce and CP) with an adjustment for dietary

		rumen undegradable (U) fraction and fractional degradation rate (kd) of D].	for-to-con ratio. H_2 pool adjusted for microbial growth on AA or NH_3-N, and for BH of uFA.
OverseerFM (Wheeler *et al*., 2008) – New Zealand. Type 2 model.	DM digestibility, ME and N of pastures and supplements. Animal ME requirement from feeding standards (mostly CSIRO, 2007).		EF (21.6 g CH_4 kg^{-1} DMI) × animal intake (IPCC, 2006; Ministry for Primary Industries, 2019).
Whole Farm Model (WFM) (Beukes *et al*., 2010) – New Zealand. Type 3 model.	Soluble ash, Ce, HC, SC, uFA, starch, large particles in the rumen, lignin, insoluble protein, AA, ammonia.	Microbial biomass and microbes associated with starch and (Ce + HC) fermentation. Ruminal acetate, propionate, butyrate and lactate.	Enteric CH_4 calculation based on H_2 balance from H_2 formation from CHO and AA fermentation, microbial growth, BH of uFA, and VFA profile.
Arla Carbon tool, Arla Foods – Sweden / Denmark / Germany / United Kingdom. Type 2 model.	GE intake, either specified by the farmer or calculated based on NorFor for cows and IPCC (2006) for heifers and bulls, and FA.	Digestibility coefficients: DM, CP, CF, structural and non-structural carbohydrates, FA, DE.	Empirical equation (IPCC, 2006).
NorFor (Nielsen *et al*., 2013) – Sweden / Denmark. Type 2 model.	DMI and dietary FA and NDF.		Empirical equation (Nielsen *et al*. 2015).
$SIMS_{DAIRY}$ (del Prado *et al*., 2011) – UK. Type 2 model.	DMI (g kg^{-1} BW d^{-1} and kg d^{-1}), C18:2 (quantity of linoleic acid in the diet), quantity of FA with a chain length ≥ 20 C in the diet.		Empirical equation (Giger-Reverdin *et al.*, 2003).
Farmscoper (Gooday *et al*., 2014) – UK. Type 2 model.	DMI, ME.		Empirical equation (IPCC, 1996), using default coefficients derived for Western Europe.
AgRE Calc – UK. Type 2 model.			Enteric CH_4 emissions for different livestock classes from IPCC Tier 2 (IPCC, 2006).

Abbreviations: AA: amino acids; AAT: amino acids absorbed from the small intestine; BH: biohydrogenation; Ce: cellulose; CF: crude fibre; CHO: carbohydrate; CP: crude protein; aNDFom: neutral detergent fibre assayed with heat stable amylase and expressed exclusive of residual ash; DE: digestible energy; DMI: dry matter intake; DOMI: digestible organic matter intake; EE: ether extract (i.e., crude fat); EPD: effective protein degradability; FA: fatty acids; FL: feeding level; FOM: fermentable organic matter; GE: gross energy; GEI: gross energy intake; HC: hemicellulose; iNDF: indigestible neutral detergent fibre; kd: fractional degradation rate; kp: fractional passage rate; ME: metabolisable energy; N: nitrogen; NDF: neutral detergent fibre; NE: net energy; NFC: non-fibre carbohydrates [calculated as DM – (ash + CP + EE + NDF)]; NFE: nitrogen free extract [calculated as DM – (ash + CP + EE + CF)]; OM: organic matter; OMD: organic matter digestibility; OMI: organic matter intake; PBV: protein balance in the rumen; PC: proportion of concentrate in the diet; pdCP: potentially digestible CP; pdNDF: potentially digestible NDF; uFA: unsaturated FA; VFA: volatile fatty acids; WSC: water soluble carbohydrates.

427 **Table 2**. Summary of the approaches used for estimating methane (CH_4) and nitrous oxide (N_2O) emissions from manure (including urine and faeces
428 deposited during grazing) and feed characteristics captured in selected on-farm models.
429

Model (source) and country	Manure CH_4 (including faeces from grazing)	Manure N_2O (including urine and faeces from grazing)	Feed characteristics captured in the model
FASSET (Olesen *et al*., 2002) – Denmark.	Does not include estimates of manure CH_4.	Estimates manure N_2O using semi-empirical equations that calculate nitrification and denitrification, and partition the end-products into N_2 and N_2O.	Dietary N.
FarmGHG (Olesen *et al.*, 2006) – Denmark.	IPCC Tier 2: calculates annual CH_4 EF based on VS excretion, B_0, and MCF (for three housing and four storage systems) but uses country specific values and also includes temperature and storage time functions.	Estimates N_2O for three housing and four storage systems as a function of temperature and/or storage time and/or tank surface area.	Dietary N.
Valio Carbo® Farm calculator – Finland.	Algorithm by Sommer *et al*. (2004) and applying experimentally derived parameters for stored slurry (Elsgaard *et al*., 2016; Petersen *et al*., 2016).	EF used for calculation of N_2O from EMEP/EEA (2016) and IPCC (2006) (Grönroos *et al*., 2017).	Total N, VSD, ash, water, P, TAN, FOM, K.
FarmSim (Salètes *et al*., 2004; Graux *et al*., 2011) – France.	IPCC Tier 2 for the calculation of CH_4 emissions from manure and housing systems.	Field: N excreta related to energy needs and diet quality, and C:N ratio of manure. Soil temperature and humidity in a dynamic equation. Barn: IPCC Tier 2 for N_2O from manure and croplands.	OMD, OM, ME and N.
INRA Method (Eugène *et al*., 2019) – France.	Annual CH_4 EF per animal based on VS excretion (from indigested OM and urinary OM, and IPCC Tier 2), B0, MCF, and MS. Annual manure EF per head: VS × EC × 365.	Eugène *et al*. (2019) does not describe N_2O approach, but recommend estimations of faecal and urinary N, along with determination of OMD and N digestibility.	OMD, OM, ME and N.
GAS-EM (Haenel *et al*., 2020) – Germany.	IPCC Tier 2: calculates annual CH_4 EF per head of animal based on VS excretion, B0, MCF, and MS. VS excretion for dairy cows based on DMI, DOM and ash in feed. Country specific values for MCF for different manure storage systems.	Type 1+ with fixed N_2O and NH_3 EF disaggregated for different manure and storage types and IPCC default for indirect N_2O from N leaching.	GE, ME, NEL, OMD, ash and N for key livestock categories
The GHG model (O'Brien *et al.*, 2010) – Ireland.	Type 1+ with fixed CH_4 EF disaggregated for storage (slurry, manure, silage effluent) or soil applied (monthly slurry, manure).	Type 1+ with fixed N_2O EF disaggregated for storage (slurry, manure) or soil applied (urine, faeces, slurry, manure), plus grazing Nex.	Total DMI, OMD, and CP of the diet.
DairyWise (Schils *et al.*, 2007; Bannink *et al*., 2020) – Netherlands.	Type 1+ with a fixed CH_4 EF for manure storage and one for manure applied to land.	Type 1+ with a fixed N_2O EF for stored manure and EF based on soil type and water level for manure N inputs to soil; and fixed fractions for N leaching and ammonia volatilisation.	Total DMI, OMD, and CP of the diet.

Dairy Tier 3 (Bannink *et al*., 2018) – Netherlands.	IPCC Tier 2: it calculates annual CH_4 EF per head of animal based on VS excretion, B0, MCF, and MS. VS excretion based on OMD and VSD. Use of a Tier 3 is limited to the prediction of ND and urine N excretion (implemented), and OMD and VS excretion (currently not implemented).	IPCC Tier 2 with EF for urine, faeces and manure storage and land application. IPCC Tier 3 for dairy cattle with prediction of Nex in urine based on N intake, apparent faecal N digestibility and N retention in animal product. Nex = N intake – N retention for all other animal classes.	Tier 2: total DMI, ME, OMD, and CP of the diet. Tier 3: DMI, aNDFom, starch, sugars, CP, non-ammonia CP, crude fat, ash, organic acids (for silages, lactic acid and VFA). *In situ* degradation of aNDFom, starch and CP [washable (W), potentially degradable (D), and rumen undegradable (U) fraction, and fractional degradation rate (kd) of D].
OverseerFM (Wheeler *et al*., 2008) – New Zealand.	CH_4 from anaerobic ponds and solids storage, application of stored manure to land, and faeces from grazing livestock. Based on proportion of faecal DM in each component and uses NZ inventory EF and IPCC Tier 2.	Estimates Nex based on DMI, dietary CP, and N in product; then splits between urine and faeces based on dietary N. Proportions urine and faeces to MMS and applies N_2O EF from the NZ inventory.	Total DMI, OMD, ash, CP.
Whole Farm Model (WFM) (Beukes *et al*., 2010) – New Zealand.	Does not estimate CH_4 from manure, but it does estimate OMD.	Does not estimate N_2O from manure, but it does estimate N excretion in faeces and urine (g N d^{-1})	Total CP intake.
Arla Carbon tool, Arla Foods – Sweden.	Emissions of CH_4 from manure is calculated based on IPCC (2006).	N_2O emitted from manure based on the amount of N in excreta. Animal-N balance. Total N_2O from manure systems calculated as the sum of direct and indirect N_2O emissions.	Total CP intake and VS, in addition to DM, CP, CF, FA, DE, NE. GE is calculated.
SIMSDAIRY (del Prado *et al*., 2011) – UK.	CH_4 from manure in storage based on IPCC, and manure on land from country specific EF (per animal) derived from Chadwick and Pain (1997) and Yamulki *et al*. (1999) for applied manure and faeces from grazing.	N_2O from manure storage from EMEP/CORINAIR (2005). N_2O from Nex deposited on soil estimated from mechanistic approach (nitrification and denitrification). Urinary and faecal N split based on dietary N.	Total DMI, OMD, ash, CP.
Cool Farm Tool (Hillier *et al*., 2011) – UK.	IPCC Tier 2: calculates annual CH_4 EF per head of animal based on VS excretion, B_0, MCF, and MS. Uses IPCC range of MMS and animal categories. Country-specific (rather than IPCC) EF for manure composting.	IPCC Tier 2: calculates annual N_2O from MMS using IPCC N excretion rates for 'animal category by region'. Uses IPCC range of MMS and animal categories. Country-specific (rather than IPCC) EF for manure composting.	Total DMI, OMD, ash, CP.
Farmscoper (Gooday *et al*., 2014) – UK.	IPCC Tier 2 (IPCC, 1996).	IPCC Tier 2 (IPCC, 1996) but with NH_3 and N leaching losses calculated in the model.	Total DMI, OMD, ash, CP.
AgRE Calc – UK.	IPCC Tier 2: calculates annual CH_4 EF per head of animal based on VS excretion, B_0, MCF, and MS.	IPCC Tier 2: calculates annual N_2O from manure based on livestock numbers, Nex/head, MS, and N_2O EF for each MMS.	Total DMI, OMD, ash, CP.

Abbreviations: B0: maximum CH_4 producing capacity of manure; Faecal DM: faecal dry matter (estimated from DMI and OMD); FOM: fermentable organic matter; MCF: CH_4 conversion factor for each MMS (by climate); MMS: manure management system (including grazing); MS: fraction of livestock handled in different MMS; Nex: N excretion (estimated based on DMI as used for enteric CH_4, N concentration of the diet and N removal in products); OMD: organic matter digestibility; TAN: total ammoniacal N; VS: volatile solids (estimated based on OMD and ash concentration of feed); VSD: volatile solids digestibility.

6. Capturing the effects of diet on emissions from ruminant systems using on-farm GHG models

6.1 Opportunities

Most prediction models of GHG emissions are based on feed (DM or GE) intake derived from feed evaluation systems applied in practice. Although these models consider the main driver of enteric CH_4 emissions, they are inadequate to capture the effect of dietary chemical components and dietary chemical/physical characteristics on GHG emissions. As a result, these models cannot capture the effect of potential dietary GHG abatement options that alter diet characteristics such as lipid (Grainger and Beauchemin, 2011), fibre (Niu *et al.*, 2018), and starch and sugar concentrations (Hindrichsen *et al.*, 2005), ruminal and whole tract digestibility (Appuhamy *et al.*, 2016), or secondary plant metabolites (Jayanegara *et al.*, 2012; Sauvant *et al.*, 2018). As a consequence, there is an increasing demand for models that take into account feed properties that both improve GHG prediction and can capture nutritional mitigation strategies (Niu *et al*., 2018; van Lingen *et al*., 2019; Benaouda *et al.*, 2019).

A close examination of several enteric CH_4 prediction equations for dairy cows used in on-farm GHG models showed that equations based on important aspects of diet composition performed better (i.e., having a greater accuracy) than those based on simpler, generic parameters or Type 1 / 2 equations (Ellis *et al.*, 2010). These findings are in agreement with the widely spread notion that enteric CH_4 production is primarily driven by both amount and composition of feed consumed. More specifically, equations that included important aspects of diet composition, such as carbohydrate components [non-structural carbohydrates (NSC), hemicellulose (HC)

458 and cellulose (Ce) (Moe and Tyrrell, 1979)] were more accurate in their predictions
459 of enteric CH_4 emissions compared with other equations (Ellis *et al.*, 2010). The Moe
460 and Tyrrell (1979) equation was used in an early version of the Molly model
461 (Baldwin, 1995) to predict CH_4 emissions (Palliser and Woodward, 2002). Ellis *et al*.,
462 (2010) examined other equations including those of Blaxter and Clapperton (1965)
463 (also tested in Molly), Kirchgessner *et al*. (1995) used in FarmGHG, Giger-Reverdin
464 *et al*. (2003) used in $SIMS_{DAIRY}$, Corré (2002) used in Schils *et al*. (2005), Schils *et al*.
465 (2006) used in DairyWise (recently updated based on Bannink et al., 2020), and a
466 Type 1 (Tier 1) and a Type 2 (Tier 2) model from IPCC (1996), used in FarmSim and
467 Phetteplace *et al*. (2001), respectively.

468 Due to the inclusion of diet composition information, the Moe and Tyrrell (1979)
469 equation was the best performing in a direct comparison with other empirical
470 equations (Ellis *et al*. 2010), as most of these equations did not include such
471 information. Although the Moe and Tyrrell equation includes some important aspects
472 of chemical composition (and an indirect estimate of feed intake level), other dietary
473 characteristics that have proven effective in CH_4 mitigation (i.e., lipid, starch and fibre
474 concentration, OM digestibility; Dijkstra *et al.*, 2010; Bannink *et al.*, 2016), are not.
475 Furthermore, the equation assumes a constant CH_4 yield per unit of NSC, HC and
476 Ce, as discussed in Ellis *et al*. (2008). The implications of this assumption is that it
477 excludes differential ruminal fermentability and passage rate of these components
478 associated with variations in feed intake level, in turn affecting efficiency of microbial
479 synthesis, VFA production, ruminal pH, VFA profile and CH_4 production (Hindrichsen
480 *et al.*, 2005; Dijkstra *et al.*, 2010). Overall, the use of fixed CH_4 conversion factors led
481 to low CH_4 prediction accuracy and imposes severe limits to opportunities for
482 nutritional mitigation of GHG emissions (Ellis *et al.*, 2010). Consistent with these

findings, Jentsch *et al*. (2007) concluded that a major component of CH_4 production could not be explained solely by DMI. Consideration of all digestible nutrients in the diet revealed that the carbohydrate fraction, particularly digestible (crude) fibre and digestible N-free residuals contributed the most to CH_4 production, whereas digestible fat had an inhibitory effect (Jentsch *et al*., 2007).

More recently, Niu *et al*. (2018) identified the main predictor variables of dairy CH_4 production (g CH_4 cow^{-1} day^{-1}), and examined the trade-offs between the availability of input variables (including diet characteristics) and the accuracy of models (assessed with several measures of model predictive ability) using the large dairy CH_4 database from the international collaborative initiative GLOBAL NETWORK (https://globalresearchalliance.org/research/livestock/collaborative-activities/global-research-project/). Along with records of enteric CH_4 production, milk yield, milk composition and BW, the database includes dietary concentrations of GE, CP, EE, NDF, ash and measured (or estimated) DMI. In addition to supporting the well-established notion that DMI is the most important variable to predict CH_4 production from dairy cows, the inclusion of diet characteristics such as NDF and EE concentration improved the accuracy of prediction of enteric CH_4 production (Ramin and Huhtanen, 2013; Niu *et al*., 2018).

The GLOBAL NETWORK project data were also used by Benaouda *et al*. (2019) to examine the predictive ability of existing enteric CH_4 equations compared with measurements obtained from calorimetry chambers, the SF_6 tracer technique and automated head chambers across ruminant species. Enteric CH_4 emissions (g CH_4 d^{-1}) from dairy cattle were suitably predicted by equations that included feed intake (DMI, GEI) and/or feed level (DMI/BW) as predictors (Mills *et al.*, 2003; Ramin and

507 Huhtanen, 2013; Charmley *et al.*, 2016). However, the best performing equation
508 (Ramin and Huhtanen, 2013) included GE digestibility and lipid concentration (EE),
509 in addition to feeding level (Benaouda *et al.*, 2019). Although most equations that
510 include digestibility use digestible OM rather than digestible GE, both variables have
511 been well established predictors of enteric CH_4 emissions (Blaxter and Clapperton,
512 1965; Sauvant and Nozière, 2016).

513 Ellis *et al*. (2010) showed that the accuracy of enteric CH_4 predictions using a fixed
514 CH_4 energy conversion factor was low. In addition to limiting the possibility of
515 implementing nutritional mitigation strategies (as mentioned above), the use of such
516 fixed conversion factors can potentially introduce substantial error at the farm scale.
517 These errors can escalate at larger scales (e.g. in GHG inventories) and may lead to
518 unsuitable mitigation recommendations or inaccurate projections of CH_4 emissions
519 over time (Bannink *et al.*, 2011).

520 The effect of dietary strategies on N_2O emissions are largely driven by total N intake,
521 or more importantly, the total N output in excreta or manure. Dietary N concentration
522 is therefore a key parameter that needs to be captured, as is the case in most on-
523 farm GHG models. In addition, the partitioning of N between urine and faeces affects
524 N_2O emissions, as it is well-accepted that N_2O emissions from urine are greater than
525 those from faeces (IPCC, 2019). Diet characteristics that affect N partitioning in urine
526 and faeces include, amongst others, DMI, N intake, rumen-fermentable OM leading
527 to the synthesis of microbial N, DM digestibility, CP concentration, and the presence
528 of secondary metabolites such as tannins. Dry matter digestibility and CP are
529 negatively related to N partitioning in faeces, whereas tannin concentration is
530 positively related to the proportion of N excreted as faecal N (de Klein and Eckard,

2008; Sauvant *et al*., 2014). All the on-farm GHG models reviewed in this paper capture DMI, dietary DMD and CP (or N) concentration, but very few (if any) take account of more detailed aspects such as the effect of differing profiles of N disappearance (ruminal and whole-tract) or the concentration of plant secondary metabolites such as tannins in the diet.

In a meta-analysis by Sauvant *et al*. (2014), relationships between CH_4 and urinary outputs were derived for ruminants fed forages (temperate and tropical forages) as their sole diet. It was shown that CH_4 production was closely related to digestible OM intake when both variables were expressed per unit of DMI or LW. This suggests that digestible OM intake is a key parameter to be captured in models for estimating CH_4 emissions from forage-fed ruminants. In agreement with these findings, Warner *et al*. (2017) reported that enteric CH_4 methane emissions were clearly affected by grass silage quality (based on harvesting leafy to late-heading grass maturity stages), more so than by DMI level (based on stage of lactation). Per unit of OM or NDF digested, CH_4 yields were similar between DMI levels, but noticeable increases were seen when reported on a digestible OM intake basis (Warner *et al*., 2017). Sauvant *et al.* (2014) also showed that, when animals are managed indoors with an anaerobic slurry storage, mitigation of enteric CH_4 appeared to be partly offset by a higher production of CH_4 from manure.

The use of dynamic mechanistic modelling in the simulation of enteric CH_4 emissions and N_2O emissions from animal excreta, has resulted in more accurate predictions than simple regression equations (Benchaar *et al.*, 1998). Although the INRA/IPCC (2006) ratio for enteric CH_4 emissions was close to unity and estimates did not differ between models for adult cows (i.e., most cattle in France), the use of dietary

555 characteristics such as digestible OM intake (corrected for feeding level and
556 proportion of concentrate in the diet) in the prediction allows for different mitigation
557 strategies to be tested (Sauvant *et al.*, 2018; Eugène *et al.*, 2019). Furthermore,
558 mechanistic modelling of methanogenesis in particular, has allowed for IPCC Tier 3
559 approaches to go beyond the farm scale (Bannink *et al.*, 2011; Huhtanen *et al.*,
560 2015). In addition, the use of a country-specific (i.e., Dutch studies only) Tier 3
561 approach to predict faecal N digestibility (Bannink *et al.*, 2018) resulted in more
562 accurate predictions than using feeding tables (CVB model; CVB, 2011), in particular
563 for Dutch studies for which more accurate estimates of model inputs on rumen
564 degradability of substrates were available. The over-prediction of the CVB model
565 would lead to an over-prediction of urine or ammoniacal N excretion, in turn leading
566 to biased estimations of the N mitigation potential from nutritional strategies (Bannink
567 *et al.*, 2018).

568 ### 6.2 Challenges

569 Overall, on-farm models that predict enteric CH_4 emissions are based on a few
570 animal and feed characteristics, but DMI is typically the key parameter to consider.
571 Analyses of large datasets of individual dairy cows have shown that simplified
572 equations based on DMI alone or in combination with a few feed and/or animal
573 related variables can predict mean enteric CH_4 emissions with a similar accuracy to
574 that of more detailed empirical equations (Hristov *et al.*, 2018; Niu *et al.*, 2018).
575 Although reliable for national emission inventory purposes, these approaches do not
576 allow for exploring nutritional mitigation options on specific farms.

577 Accurate predictions of DMI are essential to achieve accurate predictions of livestock
578 emissions, including enteric and manure CH_4, and N_2O emissions. In some

579 confinement-type feeding systems where predictions of DMI can rely on robust and
580 frequently-updated feed evaluation systems, the issue of prediction accuracy
581 becomes of less concern. For example, using data from North America, model
582 equations that used estimates of DMI could predict enteric CH_4 emissions as
583 accurately as when using measured DMI data, provided DMI could be estimated with
584 reasonable accuracy (Appuhamy *et al.*, 2016), and prediction accuracy was not
585 improved by further addition of diet characteristics to the model (Niu *et al.*, 2018).
586 Using European data, estimates rather than measured DMI provided for acceptable
587 predictions (RMSPE ≤15%; CCC ≥ 0.50), whereas using estimates of DMI for
588 Australia and New Zealand provided for poor predictive performance of enteric CH_4
589 emissions (RMSPE > 25%; CCC < 0.40) (Appuhamy *et al.*, 2016). The differences in
590 accuracy were most likely attributed to the DMI prediction models used, based on
591 North American data that are unlikely to address diets with a high proportion of
592 forage (Appuhamy *et al.*, 2016; Hristov *et al.*, 2018). As expected, forages (offered
593 either fresh or conserved) dominated the diets used in Australia and New Zealand
594 (mean values of 88% vs. 52% and 64% for North American and European diets,
595 respectively). Obtaining reasonable estimates of herbage DMI in a grazing situation
596 can be challenging, as results obtained from different methods (e.g., the use of
597 markers, herbage disappearance and inferences from animal performance) can vary
598 substantially and can potentially be misleading (Macoon *et al.*, 2003).

599 The type of livestock farming system is also an important consideration when
600 assessing the value of refining on-farm GHG models to capture more details
601 concerning dietary strategies. In fully housed livestock systems, where animals are
602 fed a total mixed ration for example, dietary measures to reduce GHG emissions can
603 be more easily adopted compared with systems that rely on grazing-based diets to

604 varying degrees. In reality, it is highly unlikely that one feed constituent (e.g., NDF
605 concentration) will vary while others remain unchanged, due to the inherent
606 association between diet constituents in diet formulation, but any goal-directed
607 change is easier to achieve in confinement-type diets or through supplemental
608 feeding than in grazing situations. The latter also offer dynamic changes (seasonal,
609 daily, hourly) in herbage quantity, composition, nutritive value, and animal
610 preference, which add complexity to DMI predictions from pasture-based systems.

611 Recently, Niu *et al*. (2018) highlighted the potential effects of increased intake and
612 associated effects such as increased passage rate and reduced time for ruminal
613 digesta retention, which in turn can reduce OM digestibility and CH_4 production per
614 unit of feed (i.e., a reduction in g CH_4 kg^{-1} DMI) (Van Soest, 1994). Feed intake is a
615 consequence of feed on offer, animal production demand and digestibility of
616 nutrients. In contrast with Type 3 models where the effect is captured, Type 2
617 models do not account for the effect of changes in feeding level, often expressed as
618 multipliers of maintenance energy levels (e.g., NRC, 2001).

619 Another challenge for on-farm GHG models to capture dietary strategies is the
620 accuracy and availability of input data to run the models. Availability of data and
621 transparency in the description and adoption of methodological procedures are
622 essential to make informed decisions on GHG abatement strategies, and even more
623 so when these tools are to inform policy (Hall *et al.*, 2010). The more detailed the
624 model in terms of inclusion of dietary characteristics, the higher the level of detail
625 that is required for the input and activity data. This not only includes detail on diet
626 composition (e.g., proportions of different feed types), but also on diet characteristics
627 within each ration ingredient or feed type. In many cases, the complexity of obtaining

628 or recording additional input data needs to be carefully balanced against the benefit
629 of being able to capture the effect of a given dietary strategy in the model.
630 Nevertheless, in many cases of intensive farming systems, reasonable estimates or
631 feed table values can be used as inputs, or obtained from commercial lab 'high-
632 throughput' analysis of nutritional value (e.g. Near Infra-Red Spectroscopy). These
633 estimates or feed table values can be more *generic* than detailed measurements as
634 an input, but they still offer potential to capture more of the variation in GHG
635 emissions, as these estimates are based on variation in feed chemical composition.

636 Empirical models that include commonly measured dietary inputs can be fairly
637 successful in predicting CH_4 emissions (Ellis *et al*., 2007). However, the impact of
638 mitigation strategies to reduce CH_4 emissions needs to be assessed in a more
639 integrated way, and often empirical models do not have the biological basis for such
640 assessment. Mathematical models of fermentation and digestion have become
641 extremely useful to simulate the complex digestive processes in the rumen, to
642 increase our understanding of the complexity of systems and to identify areas where
643 knowledge is lacking and more research is required to improve both understanding
644 and accuracy of predictions (Ellis *et al*., 2008). Dynamic components of CH_4
645 predictions have been added to these mechanistic models (e.g., Benchaar *et al*.
646 1998; Mills *et al*. 2001) and delivered improved prediction of the effect of specific
647 mitigation measures. However, limitations in the accuracy of CH_4 predictions
648 continue to surface (Bannink et al., 2016). Earlier work in search for causes of
649 inaccurate simulation of rumen function (leading to inaccurate predictions of enteric
650 CH_4) already identified the need for accurate estimates of stoichiometry of VFA
651 production with substrate fermentation and VFA absorption kinetics (Bannink *et al*.,
652 1997) and interspecies H_2 transfer (Ellis *et al*., 2008).

653 Finally, it is important to note that most of the models available (and those selected
654 in this review) have been developed for temperate conditions and related animal
655 breeds and feed nutritive values, often involving adult Holstein-Friesian and Jersey
656 cattle with *ad libitum* access to feed and quality drinking water (i.e., low nitrate
657 concentrations) under European and New Zealand conditions. Models have been
658 developed for diets or dietary ingredients with a common mineral, DM and OM
659 concentration including typical grass / legume mixed pastures (fresh and conserved),
660 maize (grain and silage), other grains, concentrates and by-products, with feed
661 nutritive values described in various feed tables. Development and evaluation of
662 models for livestock production systems in arid and tropical regions is extremely
663 limited to date, highlighting the need for greater effort by the international research
664 community in this area.

665 ## 7. Conclusions

666 The models reviewed in this paper generally include Type 2 or combinations of Type
667 2 and Type 3 approaches depending on livestock class, GHG considered and
668 emissions source involved. The majority of enteric CH_4 models use a Type 2
669 approach to estimate DMI from production data and animal population
670 characteristics, whereas a limited number of models use the more detailed
671 mechanistic Type 3 approach. Type 2 models can capture a varying range of diet
672 characteristics, including total DMI, DM or OM digestibility, ME/GE, and CP
673 concentration. Most models then use a CH_4 EF (g CH_4 kg^{-1} DMI) and a N_2O EF
674 (N_2O-N emitted as % of N excreted) to estimate GHG emissions. Some models
675 include different CH_4 EF for different diets or dietary ingredients (e.g., DairyWise,
676 with EF values derived from a Type 3 approach) rather than CH_4 EF purely based on

677 animal species (e.g., OverseerFM). Only Type 3 models represent underlying
678 mechanisms such as ruminal fermentation and total-tract digestive processes (e.g.,
679 Karoline, Dairy Tier 3, Whole Farm Model). Prior to a proper representation of these
680 processes, ruminal digestibility of, and competition for, different substrates, bypass
681 fractions, and the rate (faster fermentation, lesser CH_4 production) and extent of
682 fermentation, along with adequate descriptions of OM chemical composition, need to
683 be captured by these models. Other aspects such as the effect of secondary
684 metabolites on CH_4 EF also need to become apparent.

685 There are opportunities for all models to improve their ability to capture dietary
686 mitigation strategies, but the value of doing so should be carefully balanced against
687 gains in accuracy of the estimates, the need for additional input and activity data, the
688 variability actually encountered on-farm and among farms, and the need for
689 consistency between different approaches that are to be used for different purposes
690 (inventory vs. on-farm accounting vs. life cycle analysis).

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