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Nordic dairy cow model Karoline in predicting methane emissions: 1. Model description and sensitivity analysis

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ABSTRACT

Decreasing methane (CH_4) emissions is necessary both environmentally, as CH_4 has a strong greenhouse gas effect and nutritionally as CH_4 represents a loss of feed energy. Karoline is a whole dairy cow mechanistic, dynamic model predicting nutrient supply and milk production. The objectives of this study were to revise the digestion and CH_4 emissions modules of the Karoline model. In addition, a sensitivity analysis was conducted to evaluate the importance of the accuracy of input data required in predicting CH_4 emissions. Modifications were made in the equations predicting digesta passage kinetics, microbial cell synthesis, digestion in the hind-gut, and utilization of hydrogen. The Karoline model predicted similar decreases in both organic digestibility (OMD) and neutral detergent fibre digestibility (NDFD) and improvements in the efficiency of microbial nitrogen synthesis with increasing dry matter intake (DMI) as reported in the literature. The proportion of ruminal digestion of total NDFD (0.95) and fecal metabolic and endogenous output (98 g/kg DMI) also agree with the literature data. Predicted total CH_4 emissions increased with a diminishing rate by increased DMI. Predicted CH_4 emissions as a proportion of GE intake decreased linearly with increased DMI. The relationships between feeding level and CH_4 emissions (a decrease of 7.8 kJ/MJ gross energy per multiple of maintenance) were in good agreement with experimental data. The sensitivity analysis suggested that feed variables related to digestion kinetics of NDF [indigestible NDF (iNDF) and digestion rate of potentially digestible NDF] have a strong influence on predicted CH_4 emissions; for example, predicted CH_4 emissions decreased with increasing iNDF concentration. Digestion rates of starch and insoluble protein had smaller effects on predicted CH_4 emissions than NDF digestion rates. Fat had a strong negative influence on predicted CH_4 emissions (0.27 kJ/MJ gross energy per 1 g fat/kg DM). The sensitivity analysis suggested that accurate values of digestion kinetic variables are required for satisfactory predictions of CH_4 emissions with mechanistic models. Based on reliable predictions of digestibility, microbial protein synthesis and CH_4 emissions, it can be concluded that the revised Karoline model is a promising tool for predicting CH_4 emissions and understanding the underlying mechanisms.

1. Introduction

There has been significant interest in developing both empirical and mechanistic models predicting enteric methane (CH_4) emissions in ruminants. The models can be used to develop strategies mitigating anthropogenic CH_4 emissions and for national inventories of CH_4 emissions. The empirical equations vary in complexity with the simplest models based on dry matter intake (DMI) (*e.g.* Axelsson, 1949). The model by Blaxter and Clapperton (1965) included energy digestibility in addition to feeding level (FL) to predict CH_4 energy as a proportion of gross energy (GE). The model of Yan et al. (2000) based on digestible energy (DE), FL and proportion of forage in the total diet precisely predicted the CH_4 emissions of cattle fed grass-silage based diets.

Dynamic, mechanistic modeling simulates CH_4 emissions using a mathematical description of ruminal digestion and fermentation (Benchaar et al., 1998; Mills et al., 2001). Mechanistic models predicted CH_4 production more accurately than simple regression equations (Benchaar et al., 1998). They concluded that the mechanistic modeling of methanogenesis could be a valuable tool predicting CH_4 emissions in dairy cows. The Nordic dairy cow model Karoline (Danfær et al., 2006a, 2006b) predicted digestion variables with reasonable accuracy and precision (*e.g.* fecal OM output RMSPE = 0.20 kg/d; $R^2 = 0.98$). A modeling exercise based on a synthetic dataset developed by Monte Carlo simulation suggested that the Karoline model has the potential to predict CH_4

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emissions accurately (Huhtanen and Ramin, 2012). The objectives of the present study were to present an updated version of the Karoline digestion model with special emphasis on CH_4 emission modules, to conduct a detailed sensitivity analysis evaluating the importance of the input data required in mechanistic models predicting CH_4 emissions, and to evaluate the model performance in response to changes in most important factors influencing CH_4 emissions. Evaluation of the model predictions of experimental data from respiration chamber studies is published in a companion paper (Ramin and Huhtanen, in press).

2. Materials and methods

2.1. Model description

The Nordic dairy cow model Karoline is a dynamic and mechanistic model that describes digestion and metabolism in dairy cows (Danfær et al., 2006a, 2006b). The fundamental underlying principles of the Karoline model were published by Danfær (1990). It predicts the amounts of nutrients absorbed from the digestive tract and metabolized in various tissues, and milk production. Although the model was constructed to predict nutrient supply and milk production in dairy cows, it can also be used to predict absorption of nutrients in growing cattle. Components of the modules related to CH_4 emissions and revisions made in the digestion model are described below. The flow chart (Supplemental Figure S1), equations (Supplemental Table S2) and alphabetical lists of variables (Supplemental Table S3) of digestion sub-models are available online at http://www.sciencedirect.com. A list of abbreviations used is also given in Table 1.

2.2. Feed characteristics

In the Karoline model (Danfær et al., 2006a) dietary carbohydrates (g/kg DM) are divided into the following fractions: neutral detergent fibre (NDF) that is divided into potentially digestible

Table 1
List of abbreviations of parameters used in the Karoline model and sensitivity analysis.

Abbreviation	Definition
AAN	Amino acid N
AcA	Acetic acid
BuA	Butyric acid
C-iNDF	Concentrate indigestible NDF
C-pdNDF	Concentrate potentiallydigestible NDF
CH_4	Methane
CH_4-E/GE	CH_4 energy as a proportion of gross energy
EE	Ether extract
EMNS	Efficiency of microbial N synthesis
F-iNDF	Forage indigestible NDF
F-pdNDF	Forage potentially digestible NDF
FL	Feeding level
iCP	Potentially indigestible protein
ISP	Insoluble protein
LA	Lactic acid
NAN	Non-ammonia N
NDFD	NDF digestibility
NH_3-N	Ammonia N
OMD	Organic matter digestibility
peptN	Peptide N
PrA	Propionic acid
REST	Rest fraction
RMSPE	Root mean square prediction error
SP	Soluble true protein
STA	Starch
TA	Total acids
WSC	Water soluble carbohydrates

fractions of forage (F-pdNDF) and concentrate NDF (C-pdNDF) and corresponding indigestible fractions (F-iNDF and C-iNDF), starch (STA), lactic acid (LA), volatile fatty acids (VFA) [acetic acid (AcA), propionic acid (PrA) and butyric acid (BuA)] and the rest fraction (REST). Huhtanen et al. (2006) and Krizsan et al. (2012) demonstrated that the concentration of iNDF in forages is closely related to *in vivo* digestibility in sheep fed at maintenance level. Dietary crude protein (CP) is described as ammonia N (NH_3-N), free amino acids (AA), peptides, soluble true protein (SP), insoluble protein (ISP) and potentially indigestible protein (iCP; Danfær et al., 2006a). Dietary fat concentration is described as ether extract (EE) that is converted to FA using empirical equations separately for forage and concentrate EE. The equations were derived from Nordic experimental data (Danfær et al., 2006a).

$$\text{Concentrate FA}(\text{g/kg DM}) = 0.904 \times \text{Concentrate EE} - 3.6 \quad (1)$$

$$\text{Forage FA}\ (\text{g/kg DM}) = 0.484 \times \text{Forage EE} - 1.3 \quad (2)$$

The REST is calculated as a difference between organic matter (OM) and the sum of NDF, starch, LA, VFA, CP and EE. It is a heterogeneous fraction including different components such as water soluble carbohydrates (WSC), pectin, plant organic acids and alcohols produced in silage fermentation.

2.3. Digestion kinetics

Digestion of dietary components in the rumen is described by the first-order kinetics. Feed specific digestion rates are used for the following components: F-pdNDF, C-pdNDF, ISP and STA. Digestion rates of these components from different ingredients are aggregated as described by Danfær et al. (2006a) into one general rate for the concentrate and forage components, respectively. The intrinsic pdNDF digestion rate (k_d; 1/h) is adjusted to account for the negative effects of increased dietary non fibrous carbohydrates (NFC) concentration as described by Danfær et al. (2006a).

$$\text{Diet adj. (fraction of 1.0)} = e^{[-0.28\times(\text{NFC/NDF})^{2.4}]} \quad (3)$$

A second adjustment factor accounting for the effects of FL, expressed here as NDF intake per g/kg of body weight (BW), on k_d (1/h) was also introduced. The effects of the slower initial rate of digestion (sigmoidal pattern of pdNDF digestion kinetics) or discrete lag time on NDF digestibility are stronger with shorter rumen residence times at high feeding levels. Another alternative to model greater effects of the slower initial rate of pdNDF with decreased rumen residence time had been to use lag pool as described by Allen and Mertens (1988). For assessing the FL adjustment factor, gas production parameters were estimated by the two-pool Gompertz model for the NDF fraction of 15 grass silages. The parameters were then used in a two-compartment rumen system with non-escapable and escapable pools to predict the digestibility of pdNDF and the first-order k_d as described by Huhtanen et al. (2008). Four different rumen residence times (30, 40, 50 and 60 h; 40:60 ratio between the rumen compartments) were used to solve first-order k_d. Estimated digestion rates with different rumen residence times were expressed as a ratio of the k_d predicted with 50 h residence time. The following relationship between FL adjustment factor and the first-order passage rate k_p (1/h; reciprocal of residence time of iNDF) was estimated:

$$\text{FL adj.} = 1.291 - 18.8 \times k_p + 205.3 \times k_p^2\ (n = 60;\ R^2 = 0.99;\ \text{SE} = 0.0039) \quad (4)$$

The equation for calculating k_p is presented later (Eq. 6). Adjusted k_d to account for the extrinsic effects of diet composition and FL was calculated as:

$$\text{Adjusted } k_d(1/\text{h}) = \text{Intrinsic } k_d(1/\text{h}) \times \text{Diet adj.} \times \text{FL adj.} \quad (5)$$