

Review Article

Mathematical Prediction Equations of Methane Emission from Dairy Cattle

Mostafa Sayed Abdellatif Khattab

Department of Dairy Sciences, National Research Centre, 12622 Dokki, Giza, Egypt

Abstract

Several techniques were developed to estimate quantity of methane emissions, but these techniques are not practical at the farm conditions, so, attention were turned toward possible approaches to formulate a high accurate prediction model. Different studies were illustrated that amount digested feeds in the rumen, concentrate and roughage contents are the most important factors affecting methane production. The digestion feed in rumen and hydrogen produced could be estimated by VFA's concentration, then it could help us to estimate. The dynamic and mechanistic models can be used to estimate methane emissions from ruminants. Their accuracy in prediction of methane production could be helpful to better estimate the contribution of ruminants to total global emission of methane. They also could be used to evaluate different strategies to reduce methane losses without affecting the metabolic efficiency of the whole rumen system. In conclusion, the developed equations could accurately and rapidly predict the CH₄ production. Further *in vitro* and *in vivo* studies with a broader range of feedstuffs differing in constituents for each category are necessary to improve the accuracy and representation of the predictive equations before their practical application.

Key words: Methane, prediction model, dairy cattle, rumen metabolism, hydrogen

Citation: Mostafa Sayed Abdellatif Khattab, 2017. Mathematical prediction equations of methane emission from dairy cattle. Sci. Int., 5: 133-141.

Corresponding Author: Mostafa Sayed Abdellatif Khattab, Department of Dairy Sciences, National Research Centre, 12622 Dokki, Giza, Egypt
Tel: +201111226523

Copyright: ©2017 Mostafa Sayed Abdellatif Khattab. This is an open access article distributed under the terms of the creative commons attribution License, which permits unrestricted use, distribution and reproduction in any medium, provided the original author and source are credited.

Competing Interest: The authors have declared that no competing interest exists.

Data Availability: All relevant data are within the paper and its supporting information files.

INTRODUCTION

Methane represents one of the major greenhouse gases which contributes to global warming¹. FAO reported that agricultural activities are estimated to be responsible of 18.5% of the produced greenhouse gasses world-wide². The estimated data showed that live stock and manure contribute by 27.5% of agricultural activities contribute in gas emission (Table 1).

It has been estimated that methane produced from livestock represent 36% of total methane produced in the world. Estimates showed that an adult cattle produce 70 and 120 kg of methane/year².

METHANE PRODUCTION IN THE RUMEN

Ruminants are characterized by its ability to digest non-degradable cellulolytic materials by fermenting it in rumen (Fig. 1), depending on the anaerobic microbial community. The rumen is a unique organ characterized as an obligate anaerobic medium (no oxygen), pH ranging between (6-7), temperature of 30°C; which provide an ideal condition for its microbial habitats (bacteria, fungi, protozoa); to microbially digest consumed feeds (~ 9 h)³.

Rumen microbial population contains multiple genera and species of anaerobic bacteria (cellulolytic, hemicellulolytic, amylolytic, proteolytic, ammonia producers, vitamin synthesizers, methane producers and fungi).

Anaerobic digestion of feeds in the rumen (Fig. 2) supply the ruminant animal with energy sources as volatile fatty acids (acetate, propionate, butyrate, valerate, iso-butyrate and iso-valerate). Methane, CO₂ and H₂ are produced as secondary metabolic components.

In the rumen, carbohydrates (simple and complex) are hydrolyzed to 5- and 6-carbon sugars by microbial enzyme produced by microbial population. Sugars are fermented to VFA through multiple-step pathways that produce reducing equivalents (i.e., metabolic hydrogen), which can be summarized in the following⁴⁻⁶:

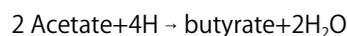
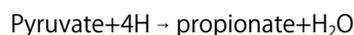
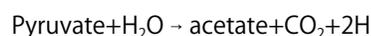
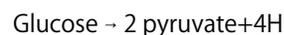


Table 1: Contribution of agricultural activities on greenhouse gases emission

Sector	Item	Contribution greenhouse gases (%)
Agriculture	Agriculture soils	6.0
	Live stock and manure	5.1
	Rice cultivation	1.5
	Agriculture use energy	1.4
	Wastewater	1.6
	Landfills	2.0
	Other	0.9

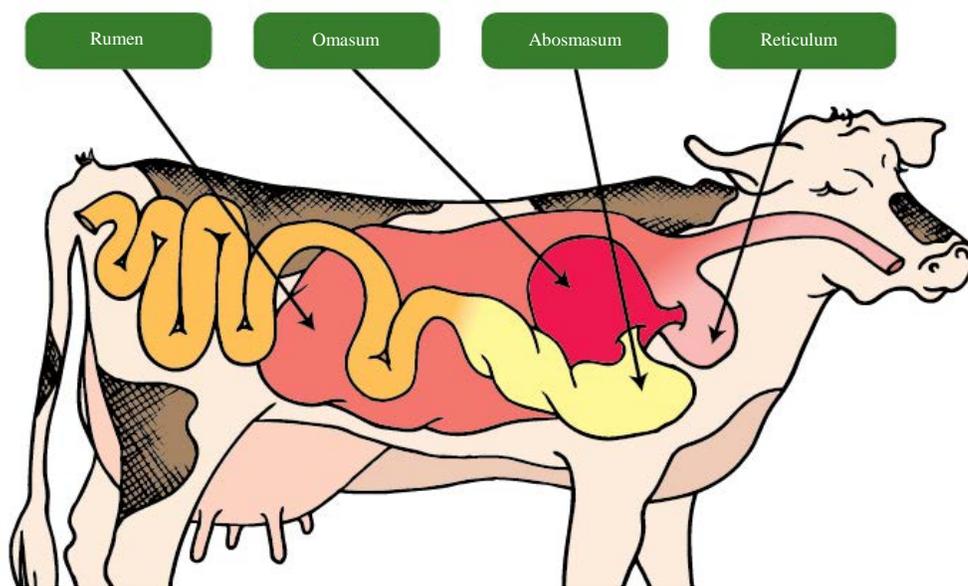


Fig. 1: Four compartment stomach of cows

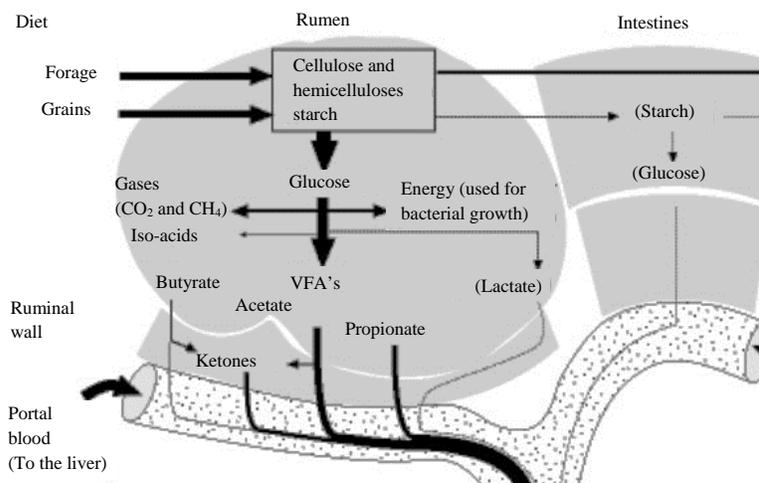


Fig. 2: Digestion of feed nutrients in the rumen

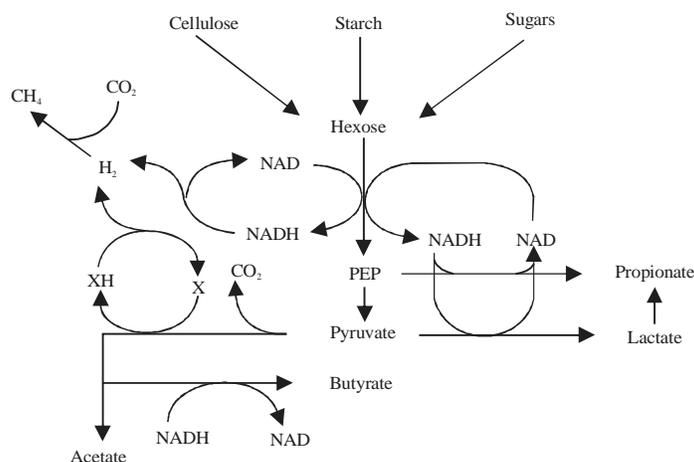
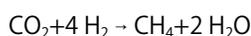


Fig. 3: Fermentation schemes of ruminal bacteria. Interspecies hydrogen transfer and hydrogen utilization by methanogens are a primary means of reducing equivalent disposal

Due to anaerobic fermentation and metabolism in the rumen, hydrogen is considered the centric metabolite, which is utilized in different metabolic pathways such as bio-hydrogenation of unsaturated fatty acids or methanogenesis⁷.

Hydrogen production occurs in three key states in the rumen, these being hydrogen gas, reduced cofactors (such as NADH and NADPH) and as free protons⁸ (Fig. 3). The major part of H⁺ produced in the rumen is utilized in bio-hydrogenation of unsaturated fatty acids consumed in the diet, while the residuals H⁺ consumed by methanogens bacteria with CO₂ and produce methane.

Methanogenesis:



PREDICTION MODELS OF METHANE PRODUCTION FROM DAIRY CATTLE

According to United Nation estimates, the world population will reach 8.9 billion habitants in 2050⁹. In this context, this contentious increase in population need parallel increase in food production, which will lead to an environmental pressure due to greenhouse gas emissions.

Different *in vitro* and *in vivo* experiments were carried out to estimate methane production from rumen fermentation under different conditions of nutritional strategies. The quantity of produced CH₄ in rumen depends on several factors such as: Daily feed intake, chemical composition, concentrate:Roughage ratio, physical properties

of diet and feed rumen digestibility¹⁰. Different studies showed that there is positive relationship between cellulolytic materials in diet and methane production; it well known that the increase of fibers in diets led to increase acetic acid in rumen and methane produced, while propionic acid was decreased^{8,10}. In the other hand, the relationship between diet concentrate content and propionic acid are negatively associated with methane production in the rumen.

Different studies have been carried out to estimate methane production in dairy cows¹⁰⁻¹⁶.

Literature illustrated that several models have been developed to maximize the accuracy of methane prediction produced in the rumen. The differences between these models are dependent on model variables, objectives and structure¹⁷⁻²¹. Different *in vitro* comparative studies were carried out to evaluate the prediction models using simulating ruminal techniques for different diets, have already been completed²²⁻²⁵.

Theoretically, prediction of methane emission could be known by the breakdown and flow of nutrients in the digestive system^{10,26}. Pathways of feed in the rumen are:

- Digested by ruminal microflora to generate volatile fatty acids (VFA's) (source of energy for ruminant) and hydrogen (H₂) as end products
- Utilized by rumen microflora for microbial biosynthesis
- The residual un-degraded feed nutrients are outflow from the rumen

Different prediction models of methane prediction in the rumen could be categorized in 2 main groups:

- Empirical (statistical) models (Regression equations)
- Dynamic and mechanistic models

Regression equation models for methane prediction:

Several regression equations were developed to estimate feed energy lost as methane by ruminants. Empirical (statistical) models that relate nutrient intake to CH₄ output directly. Different prediction equations were suggested to predict methane to elucidate the factors affecting the CH₄ output of feedstuffs or diets^{27,28}. The concept of regression equation models estimate production of methane depends on different variables such as dry matter intake (DMI), gross energy (GE) and digestible energy (DE).

Blaxter and clapperton prediction model: The equation of Blaxter and Clapperton²⁹ was derived from series *in vivo* methane measurements experiments on sheep and cattle fed

different diets. The equation depends on digestible energy and feed intake as variables relative to maintenance:

$$\text{CH}_4 = 1.30 + 0.122 \text{ D} + \text{L} (2.37 - 0.05 \text{ D})$$

Where:

D = Digestibility at the maintenance level of feeding

L = Level of feeding

Different application and evaluation trials of Blaxter and Clapperton equation showed an overestimation of methane production by 0.32 Mcal/day¹¹, this inaccurate estimation may returns to equation does not account for another important factor such as mentioned previously. Also, the equation cannot be applied to a wide range of feedstuffs varying in chemical constituents^{28,30}.

Moe and tyrrell prediction model: Moe and Tyrrell³¹ used data from cattle fed high-quality diets in order to derive their equation, which related the produced methane (Mcal/day) to some variable which were soluble residue intake (kg/day), hemicellulose and cellulose intake from cattle fed high quality dairy diets. Their regression equation for prediction methane output was:

$$\begin{aligned} \text{CH}_4 \text{ (g/day)} = & 33.0 + 104.6 \times \text{digested cellulose (kg/day)} \\ & + 38.5 \times \text{digested hemicellulose (kg/day)} \\ & + 20.5 \times \text{digested neutral detergent-soluble} \\ & \text{residue (kg/day)} \end{aligned}$$

Originally, Moe and Tyrrell³¹ meant with soluble residue a residual of subtracting crude protein and ether extract from the neutral-detergent solubles. Moe and Tyrrell³¹, reported that the produced methane of soluble carbohydrate fermentation is less than structural cell wall carbohydrates.

The accuracies of Moe and Tyrrell³¹ equation containing descriptors of dietary carbohydrate intake varies in error of prediction within unstable range of dairy cattle diets. Wilkerson *et al.*³² suggested that Moe and Tyrrell's model was a development of Blaxter and Clapperton equation, because Moe and Tyrrell incorporated feed characteristics in their equation. The variables most effective in accurately predicting methane production include the digestibilities of fiber components such as cellulose, hemicellulose and neutral detergent soluble³³.

Other evaluation and comparison studies for Moe and Tyrrell³¹ model showed that the model overestimate the prediction of methane produced in the rumen because the model because the model does not account for possible

effects of other factors ether extract content and its effect of ruminal fermentation³⁴ and lower correlation factor with *in vivo* methane measured³⁵.

Sequential prediction models: The objective of the sequential approach for prediction methane production is similar to the IPCC³⁶, which is based on different levels of available information. The major level of sequential approach was mainly, gross energy, dietary and animal levels³⁷:

- In the first level, methane are predicted using the gross energy intake
- In the second level, diet characteristics [CP (%), NDF (%), ADF (%), EE (%) and ME], as well as GEI, are potential predictors
- In the third level, milk composition (fat, protein and non-fat soluble) and animal information (body weight and breed), as well as variables from the dietary level are potential predictors

GEI was selected as a measure of animal's feed intake to be consistent and comparable with current national greenhouse gas inventories and to examine methane emissions from an energy loss perspective.

Yan *et al.*¹² developed a prediction model using more variables than used in the previous models. The developed model were carried out using a data of total 322 cattle roughage dry matter (DM) intake as a proportion of total DM intake (S_{DMI}/T_{DMI}), total acid detergent fiber (ADF) intake as a proportion of T_{DMI} (T_{ADFI}/T_{DMI}) or roughage ADF intake as a proportion of T_{ADFI} (S_{ADFI}/T_{ADFI}) and feeding level above maintenance (FL-1).

Yan *et al.*¹² were illustrated the step of creating methane prediction equation and the relationship between methane energy (CH_4-E) and energy intake and other variables on the combined data of dairy and beef cattle in four steps:

- First step, relating CH_4-E to total GE intake (GEI) and digestible energy (DE) intake (DEI) by using the linear regression technique:

$$CH_4-E = a+b \cdot \text{intake}$$

- Second step, calculated methane energy (CH_4-E/GEI , CH_4-E/DEI) from first step were then each related to feeding level (FL), apparent energy digestibility, roughage DM intake (S_{DMI}) as a proportion of total DM intake (T_{DMI}) (S_{DMI}/T_{DMI}), total ADF intake (T_{ADFI}) as a proportion of T_{DMI}

(T_{ADFI}/T_{DMI}) and roughage ADF intake (S_{ADFI}) as a proportion of T_{ADFI} (S_{ADFI}/T_{ADFI}):

$$CH_4-E/\text{intake} = a+b \cdot \text{digestibility}$$

$$CH_4-E/\text{intake} = a+b \cdot (FL-1)$$

$$CH_4-E/\text{intake} = a+b \cdot (\text{dietary factor})$$

- Third step, methane energy values calculated from second step related to energy intake (GE or DE) and FL above maintenance (FL-1) or dietary factor (T_{ADFI}/T_{DMI} , S_{DMI}/T_{DMI} or S_{ADFI}/T_{ADFI}):

$$CH_4-E = a+b \cdot \text{intake} + c \cdot (FL-1)$$

$$CH_4-E = a + \text{intake} \cdot [b + c \cdot (\text{dietary factor})]$$

- Finally, CH_4-E was predicted using the above three groups of variables {energy intake (GE or DE), feeding level (FL-1) and dietary factor (T_{ADFI}/T_{DMI} , S_{DMI}/T_{DMI} or S_{ADFI}/T_{ADFI}):

$$CH_4-E = a + \text{intake} \cdot [b + c \cdot (\text{dietary factor})] + d \cdot (FL-1)$$

Results showed two equations gave accurate prediction:

$$CH_4-E \text{ (MJ/day)} = DEI (0.094 + 0.028 S_{ADFI}/T_{ADFI}) - 2.453 \text{ (FL-1)}$$

$$CH_4-E \text{ (MJ/day)} = DEI (0.096 + 0.035 S_{DMI}/T_{DMI}) - 2.298 \text{ (FL-1)}$$

The relationship between predicted methane and actual methane were highly significant ($p < 0.001$) and R^2 values was 0.92 for each equation.

Another study for creating prediction equation of methane production was carried out by Moraes *et al.*³⁷ using database containing 2574 indirect respiration calorimetry records of dairy and beef cattle in 62 studies conducted from 1963-1995 in the former USDA Energy Metabolism Unit at Beltsville, Maryland.

Model development was conducted in a sequential approach, with increasing model complexity at each level. Researchers aimed to similar the sequential approach was similar to the IPCC³⁶, which is based on Three complexity levels namely gross energy, diet and animal levels:

- In the first level, emissions are predicted depending on the animal's gross energy intake
- In the second level, diet traits (fiber fractions, crude protein, ether extract and metabolizable energy), as well as gross energy intake are used to predict

- In the third level, milk composition (fat, protein and nonfat soluble) and animal information (body weight and breed), as well as variables from the dietary level are potential predictors

Gross energy intake was mainly selected as a measure of animal's feed consuming to be consistent and comparable and to examine methane emissions from an energy loss perspective.

Models calculated methane production (MJ/day):

$$CH_4 = 3.247 + 0.043 \times GEI$$

$$CH_4 = 0.225 + 0.042 \times GEI + 0.125 \times NDF - 0.329 \times EE$$

$$CH_4 = -9.311 + 0.042 \times GEI + 0.094 \times NDF - 0.381 \times EE + 0.008 \times BW = 1.621 \times MF$$

Results of prediction using the equation showed that gross energy intake was the important key variable in predicting methane emissions and was present in the selected models across all complexity levels and data sets.

Castro-Montoya *et al.*, mechanistic model: Recently, many efforts were carried out to investigate the correlation between ruminant animal products especially milk and the methane produced through fermentation in the rumen of the producing animals. Different studies tried to correlate between milk fatty acids (MFAs) and methane production³⁸⁻⁴³. Castro-Montoya *et al.*¹⁵ developed a model by inclusion dry matter intake (DMI) to improve the prediction of CH₄ emissions (g/day) compared with models based solely on MFAs. Results showed that combining milk fatty acids and DMI present better prediction than predictions based on DMI only. Methane emissions from lactating ruminant have been traditionally associated with MFA by regressing the former on the MFAs proportions intending to generate a prediction of the actual amount of CH₄ emitted by an animal⁴⁴.

Correlations between CH₄ and individual MFAs were generally weak through different data set has been observed in different studies^{18,40,41}.

Mohammed *et al.*⁴⁰ and Rico *et al.*⁴¹ reported that the highest correlation between CH₄ produced (g/day) and cis-9 C17:1 (Table 2).

In agreement of Castro-Montoya *et al.*¹⁵ model, Rico *et al.*⁴¹ reported that including DMI and MFA in the model was better than other model based on MFAs only (R² = 0.8 v. 0.58).

Table 2: Pearson's correlations between methane emissions and portions of individual milk fatty acids (MFA) (g/100 MFA)

Positive correlation	Negative correlation
CH₄ (g/day)	
C _{12:1} (r = 0.39)	Cis-9 C _{17:1} (r = -0.61)
Trans-15 C _{18:1} (r = 0.37)	Iso-C _{18:0} (r = -0.61)
C _{9:0} (r = 0.36)	Trans-13 C _{18:1} (r = -0.58)
CH₄ (g kg⁻¹ DMI)	
C _{16:0} (r = 0.63)	C _{17:0} (r = -0.65)
Cis-9 C _{16:1} (r = 0.54)	n-6 C _{18:3} + C _{20:0} (r = -0.63)
Cis-15 C _{18:1} (r = 0.42)	Trans-13 C _{18:1} (r = -0.56)
CH₄ (g kg⁻¹ milk)	
Cis-9 C _{16:1} (r = 0.44)	n-6 C _{18:3} + C _{20:0} (r = -0.39)
C _{16:0} (r = 0.41)	Cis-13 C _{18:1} (r = -0.39)
Trans-14 C _{16:1} (r = 0.36)	Anteiso-C _{17:0} (r = -0.40)

The Castro-Montoya *et al.*¹⁵ model approach depended on multiple linear regression by using data set (n = 140).

The regression analysis was done by fitting a generalized linear mixed model, which deals with correlations from repeated measurements and/or shared random effects from an experiment⁴⁵:

$$CH_4 \text{ (g/day)} = 471 - 137 \times \text{cis-13 C}_{16:1} - 824 \times \text{trans-14 C}_{16:1} + 138 \times \text{trans-10 C}_{18:1} - 280 \times \text{trans-12 C}_{18:1} - 325 \times \text{trans-11, cis-15 C}_{18:2}$$

$$CH_4 \text{ (g/day)} = 282 + 16.6 \times \text{DMI} - 89 \times \text{C}_{17} - 32.3 \times \text{trans-C}_{18:1} - 146 \times \text{cis-13 C}_{16:1} - 117 \times \text{iso C}_{17:0}$$

Nevertheless, two main weaknesses could be identified in previous studies: First, models have been developed depending on limited number of observations or from experiments including treatments directly influencing the MFA profile potentially holding a powerful relation with CH₄ emissions.

Second, models were not validated on experiments to evaluate if it could determine coefficients reflect the variation explained by MFAs as well as random effects of experiment¹⁵.

Moreover, Milk fatty acid might be an alternative high characterize from low emitters. The key factor of utilizing MFAs as effective variable is their distribution profile, rather than their concentrations^{46,47}.

From current approaches, milk fatty acids appear to have a little potential to predict CH₄ emitted by dairy cows.

Dynamic and mechanistic models

Description of the mechanistic models: The dynamic and mechanistic for predicting models of methane production from rumen were structured on models which predict rates and patterns of nutrient absorption. The variables included in prediction models are describing soluble and insoluble

dietary nutrients, fermentation intermediates, end products, degradation rates for hemicellulose and cellulose. The rumen prediction models simulate the effect of rumen kinetics such as pH on microbial maintenance requirements, proportions of VFA produced and rates of hemicellulose and cellulose degradation⁴⁸. All that variable to help increase the prediction accuracies which based on hydrogen balance. The produced hydrogen as intermediate in the metabolism are used for microbial cell growth and production and for biohydrogenation of unsaturated fatty acids consumed in the diet. The remaining hydrogen is utilized by methanogenic archaea in reduction of carbon dioxide to methane⁴⁹.

Baldwin *et al.*, mechanistic model: As described previously, the produced methane in the rumen depends on hydrogen produced or used during the formation of VFA which could be calculated according to rumen fermentation stoichiometries⁵, the hydrogen quantities consumed in biosynthesis of microbial cell components were calculated based on equations reported by Reichl and Baldwin⁵⁰. While, the amounts of hydrogen used for saturating dietary unsaturated fatty acids consumed is calculated according to: The hydrolysis of lipid releases 1 mol of glycerol and 1.8 mol of long-chain fatty acid per mole of lipid⁵⁰.

The steps of ruminal methane production calculation are:

Amount of hydrogen resulting from fermentation of carbohydrates (H_{car}) to VFA:

$$H_{car} = (Ac_{car} \times 2.0) - (Pr_{car} \times 1.0) + (Bu_{car} \times 2.0) - (VL_{car} \times 1.0)$$

where, Ac_{car}, Pr_{car}, Bu_{car}, VL_{car} are the amounts (mol/day) of acetate, propionate, butyrate and valerate produced from fermentation of carbohydrates, respectively.

Quantity of hydrogen resulting from fermentation of amino acids (H_{aa}) to VFA:

$$H_{aa} = (Ac_{aa} \times 2.0) - (Pr_{aa} \times 1.0) + (Bu_{aa} \times 2.0) - (VL_{aa} \times 1.0)$$

where, Ac_{aa}, Pr_{aa}, Bu_{aa} and VL_{aa} are the amounts (mol/day) of acetate, propionate, butyrate and valerate produced from fermentation of amino acids, respectively.

Amount of hydrogen used for biosynthesis of microbial cell components (H_{mg}):

$$H_{mg} = (MG_1 \times -0.42) + (MG_2 \times 2.71)$$

where, MG₁ and MG₂ are the amounts of microbes (kg/day) growing with and without preformed amino acids, respectively. The coefficients -0.42 and 2.71 are moles of hydrogen kg⁻¹ of microbes.

Amount of hydrogen used for biohydrogenation of unsaturated fatty acids (H_{FA}):

$$H_{FA} = 1.8 \times Lipid_{ing} \times H_{SFA}$$

where, Lipid_{ing} is the amount of lipids ingested (mol/day) and H_{SFA} represents moles of hydrogen used for saturation of 1 mole of unsaturated fatty acids.

Calculation of hydrogen balance in the rumen:

$$H_{rumen} = H_{car} + H_{aa} - H_{mg} - H_{FA}$$

Calculation of ruminal methane production:

$$CH_{4rumen} \text{ (mol/day)} = H_{rumen} / 4.0$$

where, 4.0 is mole of hydrogen used for the production of 1 mole of CH₄

And, finally:

$$CH_{4rumen} \text{ (Mcal/day)} = CH_{4rumen} \times 0.211$$

where, 0.211 is heat combustion of methane in mega calories mol⁻¹.

The current updated model of Baldwin *et al.*⁵¹ requires more extensive feed evaluation characterization than other models such as the chemical composition of the diets especially cell walls (cellulose, hemicellulose and lignin), protein (soluble and insoluble fractions), non-protein nitrogen, starch and its solubility, soluble sugars, pectin, organic acids, lipids, lactate and VFA. One of the advantages of Baldwin *et al.*⁵¹ model is most of the variable used for prediction can be easily found in tables of feed composition or in the literature. While some other variables are scarce (pectin, organic acid concentrations). Some evaluating studies of updated Baldwin *et al.*⁵¹ model stated overestimation by 0.93 Mcal/day which could be due to an incorrect estimation of the pattern of VFA produced in the rumen¹¹.

CONCLUSION

Using prediction method for estimating methane produced from dairy cattle could be an accurately and rapidly

method to evaluate feeds and animal performance which could be helpful to create an effective strategies for reducing methane emission from livestock animals. While, further *in vitro* and *in vivo* studies with a broader range of feedstuffs differing in constituents for each category are necessary to improve the accuracy and representation of the predictive equations before their practical application.

SIGNIFICANCE STATEMENTS

- This study was carried out to review the mathematical efforts to create a prediction equation for methane production from dairy cattle
- Prediction equations need further studies to increase the accuracy of the prediction equation under different production conditions and variables

REFERENCES

1. Johnson, K.A. and D.E. Johnson, 1995. Methane emissions from cattle. *J. Anim. Sci.*, 73: 2483-2492.
2. FAO., 2006. *Livestock Long Shadow: Environmental Issues and Options*. Food and Agriculture Organization, Rome, Italy, ISBN: 9789251055717, Pages: 390.
3. Church, D.C., 1988. *The Ruminant Animal: Digestive Physiology and Nutrition*. 2nd Edn., Prentice Hall, Englewood Cliffs, New Jersey, USA.
4. Hungate, R.E., 1966. *The Rumen and its Microbes*. 1st Edn., Academic Press, London, Pages: 553.
5. Czerwaski, J.W., 1986. *An Introduction to Rumen Studies*. Pergamon Press, Oxford, Pages: 233.
6. Moss, A.R., J.P. Jouany and J. Newbold, 2000. Methane production by ruminants: Its contribution to global warming. *Annales Zootechnie*, 49: 231-253.
7. Van Lingen, H.J., C.M. Plugge, J.G. Fadel, E. Kebreab, A. Bannink and J. Dijkstra, 2016. Thermodynamic driving force of hydrogen on rumen microbial metabolism: A theoretical investigation. *PLoS ONE*, Vol. 11. 10.1371/journal.pone.0161362.
8. Hegarty, R.S. and R. Gerdes, 1999. Hydrogen production and transfer in the rumen. *Recent Adv. Anim. Nutr. Aust.*, 12: 37-44.
9. United Nations, 2004. *World Population to 2300*. United Nations Publications, New York, USA., ISBN-13: 9789211514018, Pages: 240.
10. Brask, M., M.R. Weisbjerg, A.L.F. Hellwing, A. Bannink and P. Lund, 2015. Methane production and diurnal variation measured in dairy cows and predicted from fermentation pattern and nutrient or carbon flow. *Animal*, 9: 1795-1806.
11. Benchaar, C., J. Rivest, C. Pomar and J. Chiquette, 1998. Prediction of methane production from dairy cows using existing mechanistic models and regression equations. *J. Anim. Sci.*, 76: 617-627.
12. Yan, T., R.E. Agnew, F.J. Gordon and M.G. Porter, 2000. Prediction of methane energy output in dairy and beef cattle offered grass silage-based diets. *Livest. Prod. Sci.*, 64: 253-263.
13. Mills, J.A.N., J. Dijkstra, A. Bannink, S.B. Cammell, E. Kebreab and J. France, 2001. A mechanistic model of whole-tract digestion and methanogenesis in the lactating dairy cow: Model development, evaluation and application. *J. Anim. Sci.*, 79: 1584-1597.
14. Garnsworthy, P.C., 2004. The environmental impact of fertility in dairy cows: A modelling approach to predict methane and ammonia emissions. *Anim. Feed Sci. Technol.*, 112: 211-223.
15. Castro-Montoya, J.M., N. Peiren, J. Veneman, B. de Baets, S. de Campeneere and V. Fievez, 2017. Predictions of methane emission levels and categories based on milk fatty acid profiles from dairy cows. *Animal*, 11: 1153-1162.
16. Cabezas-Garcia, E.H., S.J. Krizsan, K.J. Shingfield and P. Huhtanen, 2017. Between-cow variation in digestion and rumen fermentation variables associated with methane production. *J. Dairy Sci.*, 100: 4409-4424.
17. Sauvant, D., 1988. [Modelling of digestion in the rumen]. *Reprod. Nutr. Dev.*, 28: 33-58, (In French).
18. Dijkstra, J. and J. France, 1995. Modelling and methodology in animal science. *Proceedings of the 4th International Workshop on Modelling Nutrient Utilisation in Farm Animals*, October 3-5, 1994, Foulum, Denmark, pp: 9-18.
19. Sauvant, D., 1997. Rumen Mathematical Modelling. In: *The Rumen Microbial Ecosystem*, Hobson, P.N. and C.S. Stewart (Eds.). Chapman and Hall, London, UK., ISBN: 978-94-010-7149-9, pp: 685-708.
20. Tedeschi, L.O., D.G. Fox, R.D. Sainz, L.G. Barioni, S.R. de Medeiros and C. Boin, 2005. Mathematical models in ruminant nutrition. *Sci. Agric.*, 62: 76-91.
21. Huhtanen, P., A. Seppala, M. Ots, S. Ahvenjarvi and M. Rinne, 2008. *In vitro* gas production profiles to estimate extent and effective first-order rate of neutral detergent fiber digestion in the rumen. *J. Anim. Sci.*, 86: 651-659.
22. Ramangasoavina, B. and D. Sauvant, 1993. [Comparative validation of 3 models of ruminal digestion to predict the duodenal N microbial flow]. *Annales Zootechnie*, 42: 164-165, (In French).
23. Kohn, R.A., R.C. Boston, J.D. Ferguson and W. Chalupa, 1995. The integration and comparison of dairy cow models. *Proceedings of the 4th International Workshop on Modelling Nutrient Utilisation in Farm Animals*, October 3-5, 1994, Foulum, Denmark, pp: 117-128.

24. Bannink, A. and H. de Visser, 1997. Comparison of mechanistic rumen models on mathematical formulation of extramicrobial and microbial processes. *J. Dairy Sci.*, 80: 1296-1314.
25. Bannink, A., H. de Visser and A.M. van Vuuren, 1997. Comparison and evaluation of mechanistic rumen models. *Br. J. Nutr.*, 78: 563-581.
26. Young, K., 2013. Methane prediction by nutrient profiles in ruminal continuous cultures fed an all forage diet of Bermuda grass or annual ryegrass. Master Thesis, Graduate School of Clemson University, Clemson, SC., USA.
27. Singh, S., B.P. Kushwaha, S.K. Nag, A.K. Mishra, A. Singh and U.Y. Anele, 2012. *In vitro* ruminal fermentation, protein and carbohydrate fractionation, methane production and prediction of twelve commonly used Indian green forages. *Anim. Feed Sci. Technol.*, 178: 2-11.
28. Ramin, M. and P. Huhtanen, 2013. Development of equations for predicting methane emissions from ruminants. *J. Dairy Sci.*, 96: 2476-2493.
29. Blaxter, K.L. and J.L. Clapperton, 1965. Prediction of the amount of methane produced by ruminants. *Br. J. Nutr.*, 19: 511-522.
30. Chen, C.N., T.T. Lee and B. Yu, 2016. Improving the prediction of methane production determined by *in vitro* gas production technique for ruminants. *Ann. Anim. Sci.*, 16: 565-584.
31. Moe, P.W. and H.F. Tyrrell, 1979. Methane production in dairy cows. *J. Dairy Sci.*, 62: 1583-1586.
32. Wilkerson, V.A., D.P. Casper and D.R. Mertens, 1995. The prediction of methane production of Holstein cows by several equations. *J. Dairy Sci.*, 78: 2402-2414.
33. Knapp, J.R., G.L. Laur, P.A. Vadas, W.P. Weiss and J.M. Tricarico, 2014. Enteric methane in dairy cattle production: Quantifying the opportunities and impact of reducing emissions. *J. Dairy Sci.*, 97: 3231-3261.
34. McGinn, S.M., D. Chen, Z. Loh, J. Hill, K.A. Beauchemin and O.T. Denmead, 2008. Methane emissions from feedlot cattle in Australia and Canada. *Aust. J. Exp. Agric.*, 48: 183-185.
35. Kebreab, E., K.A. Johnson, S.L. Archibeque, D. Pape and T. Wirth, 2008. Model for estimating enteric methane emissions from united states dairy and feedlot cattle. *J. Anim. Sci.*, 86: 2738-2748.
36. IPCC., 2006. IPCC guidelines for national greenhouse gas inventories. National Greenhouse Gas Inventories Programme, Institute for Global Environmental Strategies, Japan.
37. Moraes, L.E., A.B. Strathe, J.G. Fadel, D.P. Casper and E. Kebreab, 2014. Prediction of enteric methane emissions from cattle. *Global Change Biol.*, 20: 2140-2148.
38. Chilliard, Y., C. Martin, J. Rouel and M. Doreau, 2009. Milk fatty acids in dairy cows fed whole crude linseed, extruded linseed, or linseed oil and their relationship with methane output. *J. Dairy Sci.*, 92: 5199-5211.
39. Dijkstra, J., S.M. van Zijderveld, J.A. Apajalahti, A. Bannink and W.J.J. Gerrits *et al.*, 2011. Relationships between methane production and milk fatty acid profiles in dairy cattle. *Anim. Feed Sci. Technol.*, 166: 590-595.
40. Mohammed, R., S.M. McGinn and K.A. Beauchemin, 2011. Prediction of enteric methane output from milk fatty acid concentrations and rumen fermentation parameters in dairy cows fed sunflower, flax, or canola seeds. *J. Dairy Sci.*, 94: 6057-6068.
41. Rico, D.E., P.Y. Chouinard, F. Hassanat, C. Benchaar and R. Gervais, 2016. Prediction of enteric methane emissions from Holstein dairy cows fed various forage sources. *Animal*, 10: 203-211.
42. Van Lingen, H.J., L.A. Crompton, W.H. Hendriks, C.K. Reynolds and J. Dijkstra, 2014. Meta-analysis of relationships between enteric methane yield and milk fatty acid profile in dairy cattle. *J. Dairy Sci.*, 97: 7115-7132.
43. Castro-Montoya, J.M., S. de Campeneere, B. de Baets and V. Fievez, 2016. The potential of milk fatty acids as biomarkers for methane emissions in dairy cows: A quantitative multi-study survey of literature data. *J. Agric. Sci.*, 154: 515-531.
44. De Haas, Y., J.J. Windig, M.P.L. Calus, J. Dijkstra, M. de Haan, A. Bannink and R.F. Veerkamp, 2011. Genetic parameters for predicted methane production and potential for reducing enteric emissions through genomic selection. *J. Dairy Sci.*, 94: 6122-6134.
45. Pinheiro, J.C. and D.M. Bates, 2000. Linear Mixed-Effects Models: Basic Concepts and Examples. In: *Mixed-Effects Models in S and S-PLUS*, Pinheiro, J.C. and D.M. Bates (Eds.). Chapter 1, Springer, New York, USA., pp: 3-56.
46. Mertens, B., N. Boon and W. Verstraete, 2005. Stereospecific effect of hexachlorocyclohexane on activity and structure of soil methanotrophic communities. *Environ. Microbiol.*, 7: 660-669.
47. Marzorati, M., L. Wittebolle, N. Boon, D. Daffonchio and W. Verstraete, 2008. How to get more out of molecular fingerprints: Practical tools for microbial ecology. *Environ. Microbiol.*, 10: 1571-1581.
48. Argyle, J.L. and R.L. Baldwin, 1988. Modeling of rumen water kinetics and effects of rumen pH changes. *J. Dairy Sci.*, 71: 1178-1188.
49. Ellis, J.L., J. Dijkstra, A. Bannink, E. Kebreab and S. Archibeque *et al.*, 2014. Improving the prediction of methane production and representation of rumen fermentation for finishing beef cattle within a mechanistic model. *Can. J. Anim. Sci.*, 94: 509-524.
50. Reichl, J.R. and R.L. Baldwin, 1975. Rumen modeling: Rumen input-output balance models. *J. Dairy Sci.*, 58: 879-890.
51. Baldwin, R.L., J. France, D.E. Beever, M. Gill and J.H. Thornley, 1987. Metabolism of the lactating cow: III. Properties of mechanistic models suitable for evaluation of energetic relationships and factors involved in the partition of nutrients. *J. Dairy Res.*, 54: 133-145.