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Short communication: Development of an equation for estimating methane emissions of dairy cows from milk Fourier transform mid-infrared spectra by using reference data obtained exclusively from respiration chambers

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ABSTRACT

Evaluation and mitigation of enteric methane (CH_4) emissions from ruminant livestock, in particular from dairy cows, have acquired global importance for sustainable, climate-smart cattle production. Based on CH_4 reference measurements obtained with the SF_6 tracer technique to determine ruminal CH_4 production, a current equation permits evaluation of individual daily CH_4 emissions of dairy cows based on milk Fourier transform mid-infrared (FT-MIR) spectra. However, the respiration chamber (RC) technique is considered to be more accurate than SF_6 to measure CH_4 production from cattle. This study aimed to develop an equation that allows estimating CH_4 emissions of lactating cows recorded in an RC from corresponding milk FT-MIR spectra and to challenge its robustness and relevance through validation processes and its application on a milk spectral database. This would permit confirming the conclusions drawn with the existing equation based on SF_6 reference measurements regarding the potential to estimate daily CH_4 emissions of dairy cows from milk FT-MIR spectra. A total of 584 RC reference CH_4 measurements (mean ± standard deviation of 400 ± 72 g of CH_4/d) and corresponding standardized milk mid-infrared spectra were obtained from 148 individual lactating cows between 7 and 321 d in milk in 5 European countries (Germany, Switzerland, Denmark, France, and Northern Ireland). The developed equation based on RC measurements showed calibration and cross-validation coefficients of determination of 0.65 and 0.57, respectively, which is lower than those obtained earlier by the equation based on 532 SF_6 measurements (0.74 and 0.70, respectively). This means that the RC-based model is unable to explain the variability observed in the corresponding reference data as well as the SF_6-based model. The standard errors of calibration and cross-validation were lower for the RC model (43 and 47 g/d vs. 66 and 70 g/d for the SF_6 version, respectively), indicating that the model based on RC data was closer to actual values. The root mean squared error (RMSE) of calibration of 42 g/d represents only 10% of the overall daily CH_4 production, which is 23 g/d lower than the RMSE for the SF_6-based equation. During the external validation step an RMSE of 62 g/d was observed. When the RC equation was applied to a standardized spectral database of milk recordings collected in the Walloon region of Belgium between January 2012 and December 2017 (1,515,137 spectra from 132,658 lactating cows in 1,176 different herds), an average ± standard deviation of 446 ± 51 g of CH_4/d was estimated, which is consistent with the range of the values measured using both RC and SF_6 techniques. This study confirmed that milk FT-MIR spectra could be used as a potential proxy to estimate daily CH_4 emissions from dairy cows provided that the variability to predict is covered by the model.

Key words: cattle, greenhouse gas, spectroscopy, proxy

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Increasing sustainability and profitability while reducing the environmental footprint of dairy production is, among others, a major challenge for the breeding sector. The reduction of greenhouse gas emissions is

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one of the key factors in meeting these intentions. A reliable method for obtaining CH_4 measurements on large numbers of individual cows in commercial farms is needed. Reliable measurement of CH_4 emissions from these dairy cows is time consuming and expensive; thus, the development of proxies to estimate individual emissions is warranted (Negussie et al., 2017).

Predicting daily CH_4 emissions of dairy cows from milk Fourier transform mid-infrared (**FT-MIR**) spectra is a promising approach (Dehareng et al., 2012; Vanlierde et al., 2015; Vanlierde et al., 2016). In industrial countries, milk FT-MIR spectra are already collected routinely at a reasonable cost in the context of milk recording programs. However, the existing prediction equation for daily CH_4 emissions from milk FT-MIR spectra is based on reference CH_4 measurements obtained using the SF_6 tracer technique (Vanlierde et al., 2016), which only quantifies enteric CH_4. On the another hand, recent investigations have developed similar models using the "sniffer" method to measure CH_4 emissions on a large number of dairy cows. However, results obtained did not confirm the potential to estimate CH_4 from milk FT-MIR spectra only (Shetty et al., 2017). Considering that the respiration chamber (**RC**) technique is praised as the gold standard method capable of measuring total CH_4 emitted by cattle (Hammond et al., 2016), the objective of the present study was to develop a new prediction equation based exclusively on reference data obtained from RC measurements. The robustness and relevance of this equation were tested through validation processes and the application on a milk spectral database. This work will also permit developing an equation based on the RC measurement technique, which gives predictions in an RC range as RC take into account emissions from the lower digestive tract (unlike the SF_6 technique). The ability to predict CH_4 emission from milk FT-MIR spectra will be discussed.

A total of 584 reference CH_4 measurements (400 ± 72 g/d) from 148 individual lactating cows were obtained in open-circuit RC from studies across Europe: Germany, Switzerland, Denmark, France, and Northern Ireland (the facilities used are described in Yan et al., 2000; Derno et al., 2009; Hellwing et al., 2012; Guyader et al., 2015; Grandl et al., 2016). Consequently, this data set represents different feeding regimens, climates, breeds, and feed types. Cows were housed in individual RC for a minimum of 3 d, and CH_4 production was measured for at least 2 consecutive 24-h periods while cows were fed ad libitum. Individual milk samples were taken during a.m. and p.m. milkings from the same days. The corresponding milk samples were collected and analyzed after sampling to obtain FT-MIR spectra. The a.m. and p.m. spectra were linked to a daily spectrum by a weighted average based on the a.m. and p.m. milk yields. The averaged milk FT-MIR spectra were then related to the corresponding 24-h CH_4 measurements. The reference data sets consisted of 211 data from Germany [50 Holstein (**HO**) cows, 406 ± 60 g/d of CH_4], 138 data from Switzerland [40 Brown Swiss (**BS**), 9 HO, 8 Red HO, and 1 HO × Simmental cows, 450 ± 76 g/d of CH_4], 130 data from Denmark (9 HO and 10 Jersey cows, 366 ± 64 g/d of CH_4), 81 data from France (9 HO cows, 366 ± 61 g/d of CH_4), and 24 data from Northern Ireland (6 HO and 6 Swedish Red Cross cows, 365 ± 44 g/d of CH_4). These cows were of varying parities and DIM (Table 1).

Table 1. Distribution of parity and stage of lactation of cows used to develop methane emission prediction equations based on respiration chamber reference measurements

	Parity			
DIM	1	2	>2	Total
1–50	1	28	13	42
51–100	3	5	9	17
101–150	3	8	13	24
151–200	1	9	18	28
>200	8	15	14	37
Total	16	65	67	148

To avoid any instrument interference and ensure that the milk FT-MIR spectra are comparable regardless of the spectrometer used and the date of analysis, the milk FT-MIR spectra were standardized according to the procedure described in Grelet et al. (2017). A first derivative was applied to the milk FT-MIR spectra as recommended by Soyeurt et al. (2011). The calibration process was developed from 3 spectral regions: between wavenumbers 968 and 1,577 cm^{-1}, 1,720 and 1,809 cm^{-1}, and 2,561 and 2,966 cm^{-1} (n = 289 data points). Constant (P0), linear (P1), and quadratic (P2) modified Legendre polynomials were computed from DIM the day of CH_4 measurement of the cows (Gengler et al., 1999) and applied to each wavenumber of spectra to take into account the metabolic status of cows during lactation (Vanlierde et al., 2015). The final modified spectra were based on 3 × 289 data points (867 data points). A modified partial least square (**PLS**) regression as implemented in the WINISI software (version 4.6; Foss, Hillerød, Denmark) was used.

The robustness of the calibration model was tested with a 5-group internal cross-validation procedure. Reference data were divided randomly into 5 groups, and 5 calibration models were developed by removing 1 individual group for each calibration development. Then, the removed group was predicted by the calibration model based on the 4 other groups. Moreover, as several measurements per cow are included in the database, a cow- and country-dependent external valida-