

Le Corps professoral de
Gembloux Agro-Bio Tech - Université de Liège vous prie
de lui faire l'honneur d'assister à la défense publique de la dissertation originale que

Monsieur GRELET Clément,

Titulaire d'un diplôme d'ingénieur en agriculture,

présentera en vue de l'obtention du grade et du diplôme de

DOCTEUR EN SCIENCES AGRONOMIQUES ET INGENIERIE BIOLOGIQUE,
le 14 juin 2019, à 14h00 précises (personne ne sera admis après cette heure),
en l'auditorium ZT1 (Bât. 1),
Passage des Déportés, 2, à 5030 GEMBLOUX.

Cette dissertation originale a pour titre :
« Promoting international prediction models through standardization of
milk-infrared spectra ».

Le jury est composé comme suit :

Président : Prof. Y. BECKERS, Professeur ordinaire,
Membres : Prof. H. SOYEURT (Promoteur), Dr P. DARDENNE (Copromoteur - CRA-W), Prof.
N. GENGLER, Prof. J. BINDELLE, Dr F. COLINET, M. F. DEHARENG (CRA-W),
Dr V. BAETEN (CRA-W), Dr P. BERZAGHI (University of Padova, Italie).

Summary

Analysis of milk by Fourier transform mid-infrared (**FT-MIR**) spectrometry provides a large amount of information on the physico-chemical composition of individual milk samples. Hence, it has been used for decades to predict fat, protein and lactose contents, and more recently fine milk composition, milk processing qualities and status of cows. This fast and cost-effective technology is a perfect candidate to provide new information for the management of individual cows. However, its concrete use by field organizations is still suboptimal given the difficulty of sharing data and models among spectrometers. The aim of this research was to optimize the use of FT-MIR analysis of milk with the final purpose of enabling the development of new management tools for dairy farmers.

In order to harmonize spectral responses among instruments and allow sharing of data and models, the first objective was to test a standardization method, well known from the NIR sector, in the frame of FT-MIR spectrometers dedicated to milk analysis. The possibility of standardizing such instruments was assessed by using the Piece-wise Direct Standardization (**PDS**) method and common raw milk samples constituted from the IDF norm (ISO 9622:2013 | IDF 141:2013). The performances of spectral harmonization were assessed by the transfer of a robust fat model from a master instrument into 21 slave instruments. Regressions were performed between master and each slave fat predictions, before and after PDS. The biases and the root mean square errors between the predictions decreased after PDS from 0.378 to 0.000 and from 0.461 to 0.016 (g of fat/100 mL of milk), respectively. These preliminary results showed that the PDS method permits a reduction of the inherent spectral variability between instruments and allows FT-MIR milk spectra to be merged from different sources into a common database, and the use of common models by all the spectrometers included in the constituted network.

The second objective was to ensure that models of interest with low robustness could also be transferred from instrument to instrument. The effect of standardization on network reproducibility was assessed on 66 instruments from 3 different brands by comparing the spectral variability of the slave and master instruments with and without standardization. With standardization, the standardized Mahalanobis distance (GH) between the slaves and master spectra was reduced on average from 2,656 to 14. The transfer of models from instrument to instrument was tested using 3 FT-MIR models predicting the quantity of daily methane emitted by dairy cows, the concentration of polyunsaturated fatty acids in milk, and the fresh cheese yield. The differences, in terms of root mean squared error, between master and slaves predictions were reduced after standardization on average from 103 to 17 g/d for methane, from 0.032 to 0.005 g/100 mL of milk for polyunsaturated fatty acids, and from 2.55 to 0.49 g of curd/100 g of milk fresh cheese yield. For all models, an improvement of prediction reproducibility within the network has also been observed. Concretely, the spectral standardization allows the transfer and use of multiple models on all instruments as well as the improvement of spectral and prediction reproducibility within the network. The method offers opportunities for data exchange as well as the creation and use of common models, at an international level, to provide more information for the management of dairy herds.

After ensuring the possibility of using spectral data under optimal conditions, the third objective was to concretize the development of models providing information on cow status to be used as management tools by dairy farmers. This work aimed to develop models to predict milk citrate, reflecting early energy imbalance, and milk acetone and β -hydroxybutyrate (BHB) as indicators of (sub)clinical ketosis. Milk samples were collected in commercial and experimental farms in Luxembourg, France, and Germany. Milk mid-infrared spectra were recorded locally and standardized. Prediction equations were developed using partial least square regression. The coefficient of determination (R^2) of cross-validation was 0.73 for acetone, 0.71 for BHB, and 0.90 for citrate with root mean square error of 0.248, 0.109, and 0.70 mmol/L, respectively. Finally, an external validation was performed and R^2 obtained were 0.67 for acetone, 0.63 for BHB, and 0.86 for citrate, with a root mean square error of validation of 0.196, 0.083, and 0.76 mmol/L, respectively. The results demonstrated the potential of FT-MIR spectrometry to predict citrate content with good accuracy and to supply indicative contents of BHB and acetone in milk, thereby providing rapid and cost-effective tools to manage ketosis and negative energy balance in dairy farms.

This research highlights new knowledge and possibilities regarding the harmonization of spectral format from different instruments in order to create, share and use FT-MIR models providing information for the management of dairy cows. More concretely, it contributes outputs as procedures to standardize instruments in routine and models to predict indicators of negative energy balance and ketosis to help farmers in the management of early lactation period.