Valorization of milk spectra: data mining of milk infrared spectra to assess transition success

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Abstract

The transition period is recognized as a critical phase in a cow's lactation. Poor transition can often be associated with clinical or subclinical diseases, but there is still a proportion of cows where poor transition cannot be linked to routinely measurable metabolites in milk. Also, millions of milk infrared spectra are generated in milk recording laboratories every year. These spectra contain comprehensive information about milk chemical composition. The objective of this study was to evaluate whether milk spectra can be mined in search for minor milk components that are not routinely measured in monthly milk samples and that might be potential biomarkers to assess transition success. First test day records within lactation and their corresponding spectra between 2015 and 2020 were extracted from Lactanet's database for Holstein cows in Québec, Canada. A categorical variable was created as a proxy for transition management based on the value of Transition Cow Index (TCI). ANOVA–simultaneous component analysis+ (ASCA+) was used to test the effect of the TCI category on spectral variability. In the first round of analysis, spectra of samples collected during the first two weeks of lactation (N=238,773) had the highest variability attributed to the TCI category, which peaked on 8-11 DIM at 3.02%. This variability falls to 1.41% on week 4 of lactation. Spectral variabilities attributed to the other studied factors, namely DIM and parity (2, 3+), were <1% and <0.5%, respectively. The second round of analysis included 41,464 spectra of samples collected during the first two weeks of lactation. The results of the analysis revealed that low TCI category had direct correlation with spectral features of milk fat and protein and inverse correlation with those of lactose. In addition, direct relationship was observed between spectral features that can be attributed to milk fat, protein, creatine, phosphate, sulfur containing compounds and trans fatty acids.

These findings suggest that more frequent milk sampling is needed during the first two weeks of lactation and monitoring additional minor milk components might be useful in assessing transition success. To conclude, milk infrared spectra represent a rich source of information regarding the chemical composition of milk, and they can be mined to gain insights and detect trends to assess transition success in dairy cows.

Keywords: Cow transition, FTIR spectroscopy, biomarkers.

Introduction

A good transition cow management is important as it affects the entire productive life of a dairy cow. The Transition Cow Index® (TCI) was developed by Ken Nordlund at the University of Wisconsin (Nordlund, 2006). The principle involves a 13-factor equation used to predict how much milk a cow is expected to produce during her 305-day lactation. Factors included in the equation are environmental (calving month), related to the cow (breed, parity) or related to her current (days in milk at first test, lactation start reason) or previous lactation (production, number of days dry, lactation start reason, lactation duration, last test day somatic cell score). At the cow's first test date, the actual projected 305-day milk yield is compared to this prediction. If the cow's production is exactly as predicted, the TCI is 0. If the cow produces more than predicted, the TCI will be positive; if less, then the TCI will be negative. A TCI value can be calculated for all second and greater lactation cows that are between 5 and 39 DIM at their first test day. The TCI is an objective way of evaluating the start of lactation for each cow. Since a good start to lactation is generally a promising sign for a good performance in overall lactation, an increase in the TCI suggests that cows will have a higher milk yield over the coming lactation. Generally speaking, a 100-point increase in a herd's average TCI corresponds to a milk yield increase of 93 kg of milk per cow for 305 days of production (Lactanet data, 2014).

Previous work has demonstrated that a very high proportion of 1st lactation cows have elevated milk beta-hydroxybutyrate (BHB) on their first test (Santschi et al., 2016a) indicating an excessive body reserve mobilization which could be linked to poor transition, excessive stress related to the onset of lactation, or a normal biological response. The ideal detection method for subclinical disorders in early lactation cows would be blood monitoring of specific metabolites. However, this technique is laborious, expensive, and intrusive. Recently, several studies suggested the use of milk spectral information and Fourier-transformed infrared (FTIR) spectroscopy as a metabolic profiling tool, specifically in early lactation (de Roos et al., 2007, Santschi et al., 2016a, Pryce et al., 2019). Around the world, routine testing for BHB has become a fast and inexpensive way to monitor herd-level prevalence of hyperketonaemia (Santschi et al., 2016b). It is hypothesized that routine testing of early lactation milk could therefore become an effective and affordable screening tool to identify individual cows needing specific attention. Recent studies have tried to predict specific metabolites with variable precision (Barbano et al., 2015, Pape et al., 2018, Luke et al., 2019), often by using FTIR to predict a single blood component. The present study aims at looking at overall spectral signature rather than trying to predict specific metabolites. This approach aims at screening the differences in spectral signature, and then eventually identify the possible metabolites involved, using a historical database of several hundred thousand Canadian Holstein cows, and using TCI as the classification variable to group cows based on their status.

Materials and methods

Assembly of the dataset

First test within lactation records and their corresponding spectra between 2015 and 2020 were extracted from Lactanet's database. The total number of extracted records was 238,773. A categorical factor was created, TCI_CAT, and three levels were defined for it as follow: 1) high, which contained records with TCI value $\geq$66th percentile and they represented successful transition, 2) mid, which contained records with TCI value >33rd percentile and <66th percentile and they were dropped to enhance the contrast in differences between records in the other two categories, 3) low, which contained records with TCI value $\leq$33rd percentile and they represented poor transition.

Testing the effect of the TCI category on spectral data

ANOVA simultaneous component analysis + (ASCA+) was chosen to test the effect of the TCI category on the spectral dataset. In the first round of analysis, the spectral dataset was divided into subsets according to days in milk (DIM): 5-7 DIM, 8-11 DIM, 12-14 DIM, week 3, week 4, week 5&6. The ASCA+ model contained the following factors: the TCI category, parity groups (second, third and higher) and DIM. In the second round of analysis, data and spectral records were limited to those that were collected during the first two weeks of lactation (N=41,464) and the spectral dataset was divided into subsets according to parity (i.e., all, second, third and higher).

Attributing milk components to the TCI category effect

Inspection of the loading spectrum of the TCI category factor allowed the association of specific milk components with the TCI category effect. High loadings, positive or negative, at characteristic wavenumbers of milk components were observed and were interpreted according to methodology described elsewhere (Bahadi et al., 2021).

Results and discussion

The first round of analysis revealed that milk spectra could capture more variability related to cow transition in the first two weeks of lactation (Table 1), which peaked in 8-11 DIM at 3.02%. This variability falls to 1.41% on week 4 of lactation. Spectral variabilities attributed to the other studied factors, namely DIM and parity (i.e., second, third and higher), were <1% and <0.5%, respectively. This observation means that the current first test date window of 6 weeks might not be tight enough to capture differences in milk composition between cows that do well or poorly during the transition period. To better understand these differences, the first test date window might need to be shortened to less than 6 weeks, preferably to two weeks of lactation, in order to better capture these differences in milk composition.

Inspection of the loading spectrum of the TCI_CAT variable reveals positive loadings at characteristic wavenumbers of milk fat and protein, and negative loadings at wavenumbers attributed to lactose. This observation suggests the existence of an inverse relationship between fat and protein, on one hand, and lactose, on the other hand, in milk samples belonging to either low or high TCI category. Indeed, when we inspected the means of fat, protein and lactose that were determined by the lab for the studied samples, we observed that milk samples from cows classified in the low TCI category had higher fat and protein content and lower lactose content in comparison with milk samples coming from cows in the high TCI category. In other words, TCI values had an inverse relationship with fat and protein content and a direct one with lactose content in milk samples.

In the second round of analysis, variability in minor milk components' spectral features was observed and it was attributed to differences in milk composition in samples coming from cows assigned to low and high TCI categories. These minor milk components are sulfur containing compounds, trans fatty acids, creatine, and phosphate. Hence, these components might be candidate biomarkers for monitoring transition success. In fact, sulfur containing compounds were already reported as probable biomarkers to monitor transition success in studies done on cows' blood plasma and liver (Zhou et al., 2017). In addition, trans fatty acids have already been reported in the literature as contributors to inflammation in bovine mammary epithelial cells (Rezamand and McGuire, 2011). The variability in lactose, sulfur containing compounds and trans fatty acids was highest during the first two weeks of lactation and in milk samples coming from cows in their third parity or higher. Cows that suffer from poor transition in a lactation become more susceptible to inflammation and health issues in subsequent

Table 1. Percentage of variance in the spectral data described by several factors of the ASCA+ model.

Term	5-7 D[1]	8-11 D	12-14 D	W3[2]	W4	W5&6
Parity	0.48	0.34	0.44	0.25	0.31	0.28
DIM	0.80	0.98	0.16	0.80	0.25	0.24
TCI_CAT	2.10	3.02	2.14	1.65	1.41	1.88

[1]D = Days
[2]W = Week

lactations, which might mean more variability in candidate transition biomarkers in cows with higher parities.

Conclusion

The findings of this study suggest that the first test date window might need to be shortened to less than 6 weeks and it is preferable to do the first test during the first two weeks of lactation in order to capture the differences in milk composition between cows that do well or poorly during their transition period. In addition, monitoring more minor milk components might be useful in assessing transition success. Milk infrared spectra represent a rich source of information regarding the chemical composition of milk, and they can be mined to gain insights and detect trends to assess transition success in dairy cows.

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