J. Dairy Sci. 103
https://doi.org/10.3168/jds.2019-17717

Predicting milk mid-infrared spectra from first-parity Holstein cows using a test-day mixed model with the perspective of herd management

P. Delhez,[1,2]* F. Colinet,[2] S. Vanderick,[2] C. Bertozzi,[3] N. Gengler,[2] and H. Soyeurt[2]
[1]National Fund for Scientific Research (FRS-FNRS), Brussels 1000, Belgium
[2]TERRA Teaching and Research Centre, Gembloux Agro-Bio Tech, University of Liège, Gembloux 5030, Belgium
[3]Walloon Breeding Association (awé Groupe), Ciney 5590, Belgium

ABSTRACT

The use of test-day models to model milk mid-infrared (MIR) spectra for genetic purposes has already been explored; however, little attention has been given to their use to predict milk MIR spectra for management purposes. The aim of this paper was to study the ability of a test-day mixed model to predict milk MIR spectra for management purposes. A data set containing 467,496 test-day observations from 53,781 Holstein dairy cows in first lactation was used for model building. Principal component analysis was implemented on the selected 311 MIR spectral wavenumbers to reduce the number of traits for modeling; 12 principal components (PC) were retained, explaining approximately 96% of the total spectral variation. Each of the retained PC was modeled using a single trait test-day mixed model. The model solutions were used to compute the predicted scores of each PC, followed by a back-transformation to obtain the 311 predicted MIR spectral wavenumbers. Four new data sets, containing altogether 122,032 records, were used to test the ability of the model to predict milk MIR spectra in 4 distinct scenarios with different levels of information about the cows. The average correlation between observed and predicted values of each spectral wavenumber was 0.85 for the modeling data set and ranged from 0.36 to 0.62 for the scenarios. Correlations between milk fat, protein, and lactose contents predicted from the observed spectra and from the modeled spectra ranged from 0.83 to 0.89 for the modeling set and from 0.32 to 0.73 for the scenarios. Our results demonstrated a moderate but promising ability to predict milk MIR spectra using a test-day mixed model. Current and future MIR traits prediction equations could be applied on the modeled spectra to predict all MIR traits in different situations instead of developing one test-day model separately for each trait. Modeling MIR spectra would benefit farmers for cow and herd management, for instance through prediction of future records or comparison between observed and expected wavenumbers or MIR traits for the detection of health and management problems. Potential resulting tools could be incorporated into milk recording systems.

Key words: mid-infrared spectroscopy, mixed model, milk composition, management

INTRODUCTION

Fourier-transform mid-infrared (**MIR**) spectroscopy is a valuable technique to describe the molecular structure of food materials. It involves the absorption of electromagnetic radiation by a sample at frequencies (400 to 4,000 cm^{-1}) that are characteristic of specific chemical bonds of a molecule (Van de Voort, 1992). The MIR spectroscopy provides analyses with high throughput, at low cost and on a large scale. Therefore, it is used in the dairy industry worldwide to predict major milk components (e.g., lactose, fat, protein contents, or urea) for milk quality control, milk payment, management of herds, or genetic studies (Gengler et al., 2016; International Committee for Animal Recording, 2017). More recently, studies have focused on milk MIR spectroscopy to predict other traits such as fine milk composition (Soyeurt et al., 2009; Bonfatti et al., 2011), milk technological properties (Ferragina et al., 2013; Visentin et al., 2015), body energy status (McParland et al., 2011), enteric methane emissions (Vanlierde et al., 2018), BW (Soyeurt et al., 2019), or geographical origin of milk (Scampicchio et al., 2016; Caredda et al., 2017).

Test-day models (**TDM**) model individual test-day records (i.e., repeated measurements over time that are specific to a particular testing day) such as milk yield or MIR traits records in dairy cattle. One of several

Received October 8, 2019.
Accepted February 27, 2020.
*Corresponding author: pauline.delhez@uliege.be

benefits of TDM is the ability to account for individual animal effects and for environmental factors occurring on the day of milk recording (Wiggans and Goddard, 1997). Their use in genetic evaluations has been widely explored (e.g., de Roos et al., 2004; Hammami et al., 2009; Leclercq et al., 2013). However, relatively few published studies considered the use of TDM for prediction and management purposes. For example, Mayeres et al. (2004), Caccamo et al. (2008), and Gillon et al. (2010) investigated the use of TDM to predict future daily milk, fat, and protein yields for management. Koivula et al. (2007) studied herd-management effect solutions from milk yield, fat, and protein contents and SCS TDM, and Bastin et al. (2009) explored the solutions and predictions of a TDM for milk urea.

Modeling MIR traits with TDM would have numerous benefits for herd management, such as the prediction of future records or missing lactation records, the evaluation of cow responses to herd management changes by adjusting herd factors in the model, or simulation of new records by modifying effects in the model. Decision support tools incorporating such models could help farmers to detect problems affecting individual cows or the whole herd through direct comparison between the actual and predicted traits, predict the production potential of heifers, analyze the results of dietary or environmental changes, and so on. With the increasing number of MIR traits (Gengler et al., 2016), implementing one TDM for each trait would be time and resource consuming from a workload and computational point of view. Therefore, predicting the whole milk MIR spectrum using TDM would be beneficial because of the reduction of the number of models to implement. All current and future MIR prediction equations could be applied on the modeled spectra to predict all MIR traits, without the need to do one TDM separately for each trait. Also, in some instances, using the whole spectra instead of specific MIR traits could bring more comprehensive information.

Several authors have already modeled milk MIR spectral wavenumbers using TDM for genetic purposes (e.g., Soyeurt et al., 2010; Wang et al., 2016; Rovere et al., 2019), but few have tackled the possible use for predictive and management purposes (e.g., Dagnachew et al., 2013b; Lainé et al., 2017). Therefore, the objective of this paper was to study the ability of a test-day mixed model to predict milk MIR spectra from first-parity Holstein cows with the perspective of herd management. To do so, we compared observed and predicted spectral wavenumbers and we examined predicted MIR milk components obtained using the observed versus predicted spectra. We tested different scenarios to assess the accuracy of the model when knowing more or less information about the cows.

MATERIALS AND METHODS

Modeling Data

The data used to build the model were collected from January 2012 to July 2017 by the Walloon Breeding Association (Ciney, Belgium) during the Walloon routine milk recording. A total of 467,496 test-day records from 53,781 Holstein dairy cows in first lactation within 541 herds were selected. Each record included the identification number of the cow and herd, the lactation stage (i.e., DIM), the test date, milk composition information (fat, protein, and lactose contents, SCC), the milk MIR spectrum, and pedigree data. Pedigree data contained 139,385 animals extracted from the database used for the official Walloon genetic evaluation and were limited to animals born after 1985. Milk MIR spectra were obtained by the analysis of individual milk samples on MilkoScan FT6000 spectrometers (Foss, Hillerod, Denmark) at the Comité du Lait laboratory (Battice, Belgium). Milk MIR spectra included 1,060 spectral wavenumbers expressed in absorbance and covering the absorption of light in the infrared region located from 900 to 5,000 cm^{-1}. All studied cows had at least 5 test-day records per lactation and belonged to herds with more than 10 recorded cows in first lactation on average over the studied period. Records with fat and protein contents as well as milk yield out of the limits set by the International Committee for Animal Recording (2017) were discarded (i.e., 3 L $<$ milk yield $<$99.9 L, 1.5 g/dL of milk $<$ fat $<$9 g/dL of milk, 1 g/dL of milk $<$ protein $<$7 g/dL of milk). Records within the 0.1% upper values and 0.1% lower values for lactose content as well as within the upper 0.1% values for milk somatic cells were removed. Records with DIM values higher than 563 (1% upper values) were also discarded.

Preprocessing of Modeling MIR Spectra

To remove baseline variation, the first derivative at wavenumber X was calculated on the raw spectra as the difference between the spectral wavenumber X−2 and the spectral wavenumber X+2. A total of 311 spectral wavenumbers out of the 1,060 were retained for this study, covering 3 MIR spectral regions: 933 to 1,589 cm^{-1}, 1,704 to 1,809 cm^{-1}, and 2,553 to 2,981 cm^{-1}. Some spectral regions were excluded based on the experience of the research team; these are regions that cannot be used effectively as they have low signal-to-noise ratio or little relevant chemical information (e.g., Iñón et al., 2004; Soyeurt et al., 2010; Capuano et al., 2014). Previous studies involving MIR spectra also retained similar spectral regions (e.g., Grelet et al., 2016; Vanlierde et al., 2018).

Spectral wavenumbers were standardized (i.e., centered and scaled) by subtracting the corresponding mean and dividing by the corresponding standard deviation. Then, principal components analysis (**PCA**) was carried out on the 311 standardized spectral wavenumbers. We performed standardization and PCA using the "stats" package in R (version 3.3.3; R Core Team, 2017). The PCA method extracts the information from a multivariate data set and expresses it as a set of new variables called principal components (**PC**). These PC are a linear combination of the original variables keeping the largest amount of information contained in the original data (i.e., the PC explain most of the variance of the original data, Palm, 1998). The use of PCA has multiple advantages for this study: decreasing the number of traits to reduce computational operations and the independence of PC, allowing a separate modeling without losing information about the interactions between spectral wavenumbers (Soyeurt et al., 2010). Let $\mathbf{X}_{(\mathrm{N}\times\mathrm{K})}$ be the matrix for the 311 spectral wavenumbers for the 467,496 test-day records, where N is the number of test-day records and K is the number of spectral wavenumbers. The contributions of the spectral wavenumbers to each PC are given by the eigenvectors. The amount of variance retained by each PC is measured by its eigenvalue. The PCA for $\mathbf{X}$ is expressed as

$$\mathbf{X}_{(\mathrm{N}\times\mathrm{K})} = \mathbf{Z}_{(\mathrm{N}\times\mathrm{M})} \times \mathbf{V}^{\mathrm{T}}{}_{(\mathrm{M}\times\mathrm{K})} + \mathbf{E}_{(\mathrm{N}\times\mathrm{K})}, \quad [1]$$

where M is the number of PC selected ($\mathrm{M} \leq \mathrm{K}$), $\mathbf{Z}_{(\mathrm{N}\times\mathrm{M})}$ is the matrix of the PC scores, $\mathbf{V}^{\mathrm{T}}{}_{(\mathrm{M}\times\mathrm{K})}$ is the transpose of the eigenvector matrix, and $\mathbf{E}_{(\mathrm{N}\times\mathrm{K})}$ is the residual matrix after the M PC are extracted from $\mathbf{X}_{(\mathrm{N}\times\mathrm{K})}$. The number of PC selected was based on the proportion of variance of the spectral wavenumbers explained and on the accuracy of the model.

Model

A total of M single-trait test-day mixed models were applied on the PC scores for the M selected PC (i.e., one model was run separately for each PC). Using single-trait models was preferred over a multi-trait model, because PC are phenotypically de-correlated and because of the computational advantage for large data sets. Running several single-trait models in parallel (i.e., data parallelism) is faster and less computationally demanding than running one multi-trait model, and therefore easier to implement in practice (Shallue et al., 2019). The single-trait test-day mixed model used was defined as follows:

$$\mathbf{y} = \mathbf{Xb} + \mathbf{Zu} + \mathbf{e}, \quad [2]$$

where $\mathbf{y}$ is the vector of observations (PC scores), $\mathbf{b}$ is the vector of fixed effects [including herd-test-year (**HTY**) effect, herd-test-month (**HTM**) effect, and DIM], $\mathbf{u}$ is the vector of random effects (including herd-test-day (**HTDr**) effect, additive genetic effect, and permanent environmental effect), and $\mathbf{e}$ is the vector of random residual effects. $\mathbf{X}$ and $\mathbf{Z}$ are the corresponding incidence matrices. The distributional assumption about the random terms of the model was

$$\mathrm{HTDr} \sim N\left(\mathbf{0}, \mathbf{I}\sigma^2_{\mathrm{HTDr}}\right),$$

$$\text{additive genetic} \sim N\left(\mathbf{0}, \mathbf{A}\sigma^2_g\right),$$

$$\text{permanent environment} \sim N\left(\mathbf{0}, \mathbf{I}\sigma^2_{\mathrm{PE}}\right),$$

$$e \sim N\left(\mathbf{0}, \mathbf{I}\sigma^2_e\right),$$

where $\mathbf{I}$ was an identity matrix, $\mathbf{A}$ was the pedigree relationship matrix, σ^2_{HTDr} was the variance of the herd test-day effect, σ^2_g was the additive genetic variance, σ^2_{PE} was the variance of the permanent environmental effect, and σ^2_e was the error variance. We divided DIM into 38 classes of 15 d. Mayeres et al. (2002, 2004) suggested a remodeling of the HTD fixed effect usually used in genetic models by replacing it with 3 herd-test-related effects to allow prediction of future test-day measurements for predictive purposes. These 3 effects are a fixed herd-test month-period effect, a fixed herd-test-year effect, and a random herd-test-day effect. The herd-test month-period effect and the herd-test-year effect represent the herd level and its seasonal trend and allow the prediction of future records, whereas the herd-test-day effect takes into account the effect of the herd at a specific date and is not assigned to the 2 other herd effects. In our study, we considered a simple herd-test-month effect instead of a herd-test month-period effect because the number of years considered in our study was higher. Variance components for random effects were estimated using expectation-maximization REML as described by Misztal (2018).

Spectral Wavenumbers Predictions for the Modeling Data Set

The solutions of the model were obtained using the BLUP method solved using the preconditioned conjugate gradient algorithm (Tsuruta et al., 2001; Misztal, 2018). Estimates of the fixed and random effects were used to compute the predicted scores of each PC. Then the predicted 311 MIR spectral wavenumbers (i.e., $\hat{\mathbf{X}}$

matrix) were obtained using the equation derived from [1]:

$$\hat{\mathbf{X}} = \hat{\mathbf{Z}} \times \mathbf{V}^{\mathbf{T}}, \quad [3]$$

where $\hat{\mathbf{Z}}$ is the matrix of the predicted PC scores and $\mathbf{V}^{\mathbf{T}}$ is the transpose of the eigenvector matrix of the PCA, and by adding the mean and multiplying by the standard deviation as data were standardized. For each spectral wavenumber, correlations were computed between observed and predicted values. Estimated variance components were also back-transformed to a spectral basis using the eigenvector matrix.

Spectral Wavenumber Predictions for Different Scenarios

Four new data sets, containing altogether 122,032 records from first-parity Holstein cows, were used to test the ability of the model to predict accurately milk MIR spectrum in 4 distinct scenarios with different levels of information about the cows. These new data sets had different levels of relatedness with the modeling data set. Information about each scenario and considered effect estimates for predictions are presented in Table 1.

The 2 first scenarios corresponded to common practical situations. The first scenario represented predictions of future test-day spectra for cows in production. It included cows for which all effects were known except the HTDr. Data were collected from August to early December 2017 (i.e., over a 4-mo period after modeling data). As expected, the median DIM was high (i.e., 310 d), but was within the DIM range of the modeling set. A similar scenario with the same known and unknown effects could be applicable to the imputation of missing spectral records for a cow with previous recorded spectral data. The second scenario represented predictions of records for a new cow in a known herd (e.g., the evaluation of the potential of a heifer before it produces milk). Data were collected from August to early December 2017 and included cows with no known test date (i.e., unknown HTDr) and no previous animal data (i.e., the permanent environmental effect was unknown).

The third and fourth scenarios were created based on records discarded when selecting data for the modeling data set. The third scenario included cows with permanent environment as the only unknown effect. This could represent a situation when we want to evaluate the potential of a new cow like a heifer and compare it to existing test-day records of the other cows of the herd. The fourth scenario included cows with minimal information (i.e., only the DIM effect and the genetic effect were known). Data were unrelated to the modeling set regarding cows and herds, but were collected over the same period. This scenario, rather theoretical, would represent predictions of records for farms that have no spectral data, but only pedigree information. The interest, more academic, is to see how the accuracy would evolve when very little information is known.

For each scenario, the predicted PC scores were obtained using the solutions from solving equations associated with the mixed model [2]. New data sets used had different levels of relatedness with the previous modeling data set adding scenario records. The trait values (i.e., PC scores) of the scenario records were considered unknown during solving. The pedigree was updated compared with the modeling data set to add animals related to the scenario cows (i.e., 191,685 animals in total). This strategy permitted estimation of predicted PC scores for scenario records by summing the solutions (i.e., fixed and random effect estimates) equivalent to those obtained using the modeling data. Missing effects, depending on the scenario, were set to zero. By extending the pedigree, solutions for genetic effect were automatically computed for new animals

Table 1. Description of the 4 scenarios (number of records, cows, and herds; effect estimates; and meaning)

				Effect estimate[1]						
Scenario	Records	Cows	Herds	HTY	HTM	DIM	HTDr	Gen	PE	Example of meaning in practice
1	10,057	4,246	422	X	X	X		X	X	Future or missing records for cows with previous records
2	17,025	7,035	430	X	X	X		X*		Potential of heifers or new cows
3	32,315	12,126	538	X	X	X	X	X*		Potential of heifers or new cows for a specific test date
4	62,625	7,507	414			X		X*		Cows with minimal information

[1]Crosses in the effect estimate columns indicate known estimates used to calculate the predictions of spectral data. Unknown effect estimates were set to zero. HTY = herd-test-year fixed effect; HTM = herd-test-month fixed effect; DIM = fixed effect of days in milk; HTDr = random herd-test-day effect; Gen = random additive genetic effect; PE = random permanent environmental effect.

*An asterisk means that the genetic solutions are based on parent averages. The absence of an asterisk means that the genetic solutions are based on the estimated breeding value of the cow.

with scenario records. These genetic solutions can be considered being the estimated breeding value for a cow that had previous production records (i.e., scenario 1), or parent averages derived through the pedigree in all other situations (i.e., scenarios 2, 3, and 4). The permanent environmental effect solutions were known for cows with previous production records, but were set to an expected value of zero for other cows. The predicted PC scores were back-transformed to the 311 spectral wavenumbers using the PCA eigenvectors of the modeling set (Equation [3]) followed by de-standardization. For each spectral wavenumber, correlations were computed between observed values and predicted values.

MIR Trait Predictions

To assess the usefulness of predicted MIR spectra for practical applications, fat, protein, and lactose contents in milk were predicted from observed MIR spectra and predicted MIR spectra for the modeling data set and scenarios. The prediction equations for fat, protein and lactose contents had a cross-validation R^2 of 0.99, 0.99, and 0.91, respectively, and a root mean square error of prediction of 0.06, 0.04, and 0.06 g/dL of milk, respectively. Reference values to build these equations came from the predicted phenotypes obtained using the Milkoscan FT6000 (i.e., these phenotypes were based on the MIR spectra), because no phenotypes were available from chemical analysis. This explains the high R^2 values obtained for these prediction equations. Traits predicted from observed and modeled MIR spectra were compared using correlations, descriptive statistics, and the root mean square error (**RMSE**). As a comparison, we also directly modeled milk fat, protein, and lactose contents using the TDM in Equation [2]. We compared correlations between traits predicted from observed spectra versus traits predicted from spectra modeled from a TDM with correlations between traits predicted from observed spectra versus traits modeled directly from a TDM. This way, we can compare the accuracy of using prediction equations on MIR spectra predicted from a TDM with the accuracy of directly modeling MIR traits using a TDM.

RESULTS AND DISCUSSION

Preprocessing of Modeling MIR Spectra

Several preprocessing methods exist for MIR data (Rinnan et al., 2009). We chose first derivative because in our study data were collected with different spectrometers over several years and derivative is a useful technique to remove baseline variation that may occur because of instabilities between instruments and over time (Owen, 1995). First-derivative preprocessing made data in our study conform more to normality as skewness and excess kurtosis were globally closer to zero after derivation (Figure 1; Kim, 2013). Further analyses of our data and comparison of models using derived and raw spectral data suggested that first derivative was a useful pretreatment for our study and improved accuracy of results (results not shown). Several authors who modeled MIR spectra using TDM previously did not precorrect spectral data (e.g., Bittante and Cecchinato, 2013; Wang et al., 2016; Zaalberg et al., 2019), whereas some precorrected MIR spectra using methods such as derivatives (e.g., Belay et al., 2017; Lainé et al., 2017) or extended multiplicative signal correction (e.g., Dagnachew et al., 2013a; Belay et al., 2017). Among these authors, Belay et al. (2017) indicated that spectral preprocessing improved prediction accuracy. Some authors stated that it is important to test different pretreatment methods to make the most advised choice and that pretreatment might only improve accuracy for some traits (De Marchi et al., 2011; Soyeurt et al., 2011; Mineur et al., 2017). This should be explored further.

One advantage of PCA was the reduction of spectral variables for modeling to decrease computer operations. Use of PCA to reduce spectral dimensions was also implemented in other studies on MIR spectra (e.g., Soyeurt et al., 2010; Dagnachew et al., 2013a,b; Bonfatti et al., 2017). We selected a total of 12 PC, representing 96% of the information (i.e., total variance) contained in spectral wavenumbers. Other authors (e.g., Dagnachew et al., 2013a; Bonfatti et al., 2017) indicated that even less than 1% loss of total variation could lead to loss of relevant information. However, in the present study, we considered 12 PC as an optimum between dimension reduction and model accuracy. Indeed, although 4% of the spectral variance was lost, the average correlation between observed and predicted spectral wavenumbers did not substantially increase when adding extra PC [i.e., the correlation increased by only 0.01 and 0.004 when increasing the number of PC from 12 to 23 (i.e., 99% of total variance) for modeling and scenarios, respectively; Figure 2]. Bonfatti et al. (2017) did not mention using spectral pretreatment, in contrast to the present study. When using raw spectra, a larger part of the variability may be noise and the remaining percentages may be interesting spectral variability. This might explain why even 1% loss of spectral variation might lead to loss of relevant information.

Variance Components

Figure 3 represents the percentage of total spectral variation retained by the model explained by the genetic, permanent environment, HTDr, and residual

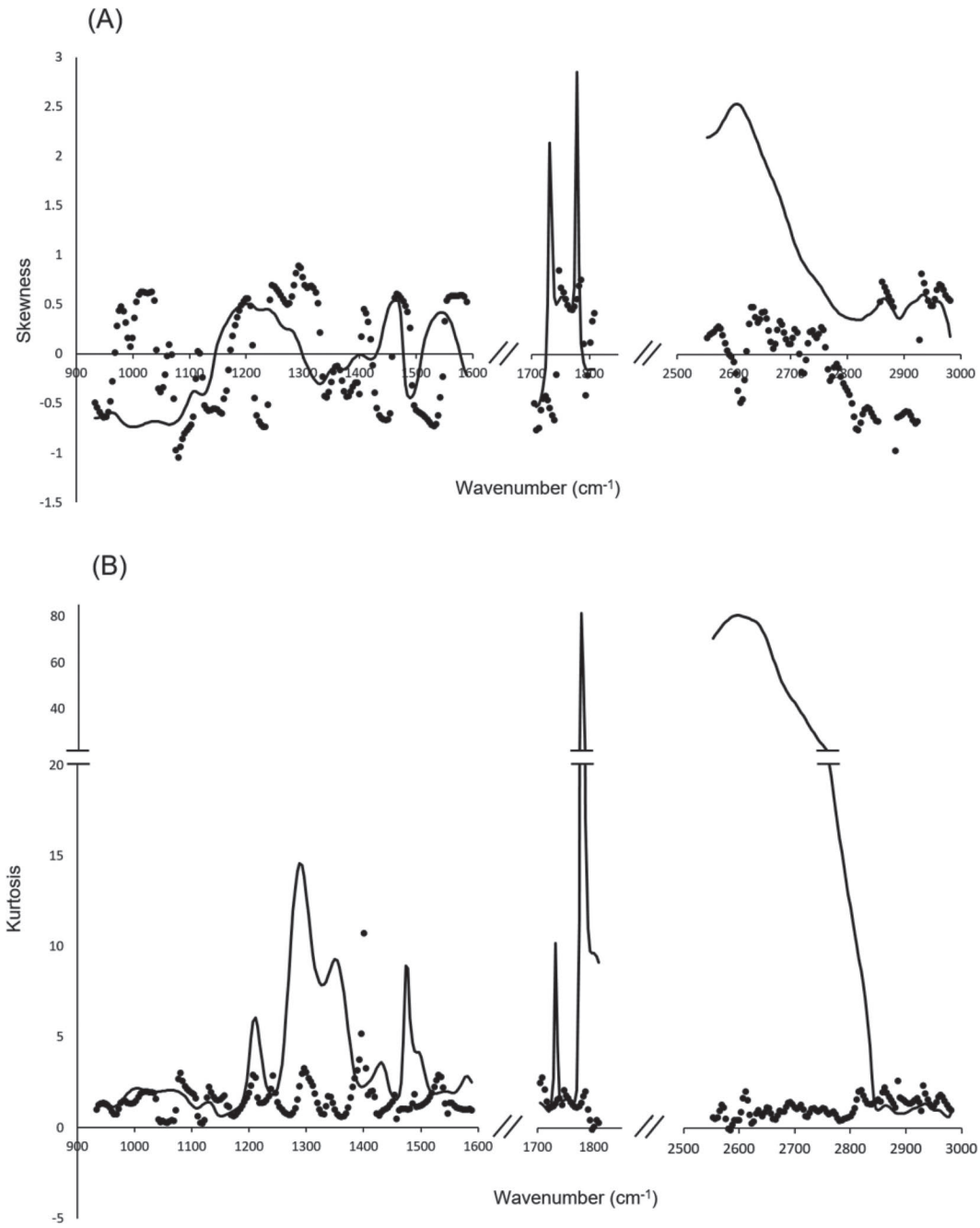

Figure 1. (A) Skewness for each of the 311 selected spectral wavenumbers for the modeling data set. The continuous line represents the raw spectra; circles represent the derived spectra. (B) Excess kurtosis for each of the 311 selected spectral wavenumbers for the modeling data set. The continuous line represents the raw spectra; circles represent the derived spectra.

effects. Genetic and residual effects explained on average, respectively, 37 and 41% of the total variation for 79% of the wavenumbers (i.e., from 933 to 1,589 cm^{-1}, 1,704 to 1,786 cm^{-1}, and 2,777 to 2,981 cm^{-1}), whereas permanent environment and HTDr explained on average 10 and 12% for the same regions, respectively. This general pattern was observed in other studies (Wang et al., 2016; Lainé et al., 2017).

In the present study, the HTDr effect was the most important effect in the spectral regions from 1,790 to 1,809 cm^{-1} and 2,553 to 2,773 cm^{-1}. Similarly, in the study of Dagnachew et al. (2013a) on dairy goat milk

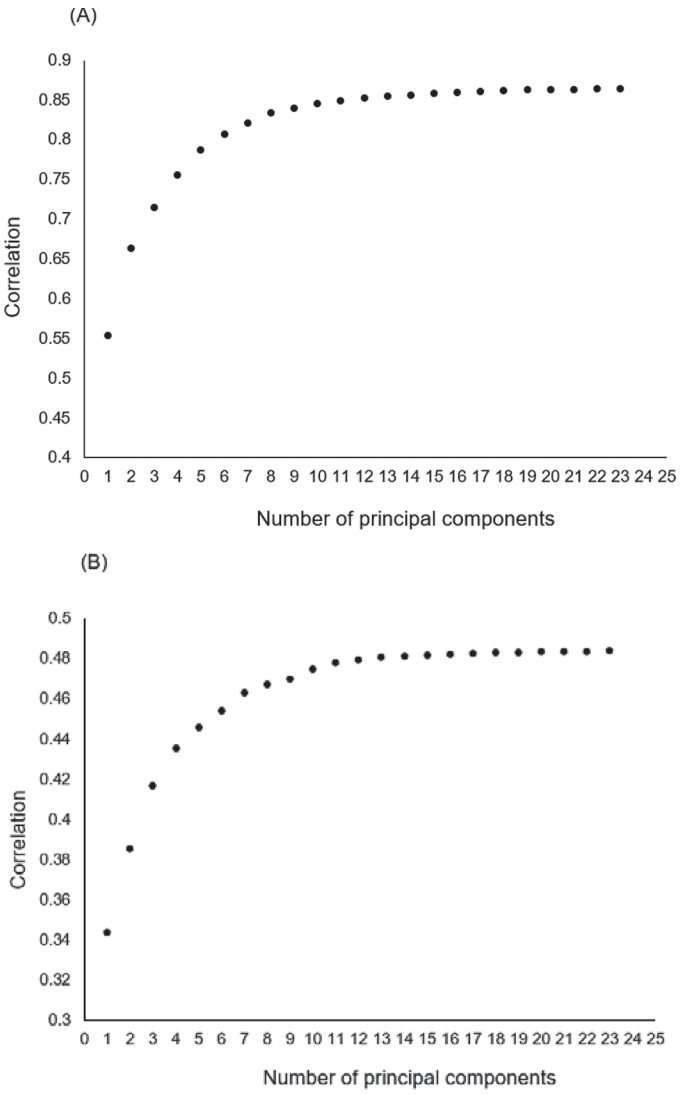

Figure 2. Average correlation between observed and predicted values for the 311 spectral wavenumbers according to the number of principal components selected (A) for the modeling data set and (B) for the 4 scenario data sets together.

spectra, HTDr also had a high variance ratio between 2,400 and 2,800 cm^{-1} and around 1,771 cm^{-1}. Wang et al. (2016) observed a lower variance ratio explained by the genetic effect around 2,400 to 2,800 cm^{-1}, which is similar to the present study. Wang et al. (2016) and Lainé et al. (2017) found a lower proportion of variance explained by the genetic effect around 1,300 to 1,500 cm^{-1}, but this was not observed in our study.

Predictions of Spectral Wavenumbers

The average correlation between observed and modeled values of the spectral wavenumbers was 0.85 for the modeling data set, the minimum correlation value was 0.67, and the maximum was 0.95 (Figure 4). Regarding the scenarios, on average correlations were the highest for scenario 3 and the lowest for scenario 4 (0.62 and 0.36, respectively), with scenarios 1 and 2 in between (0.56 and 0.37, respectively, Table 2). We observed low correlations for spectral regions from 1,790 to 1,809 cm^{-1} and from 2,553 to 2,773 cm^{-1} for scenarios 1, 2, and 4 (Figure 5). When removing these regions, the first scenario (i.e., prediction of future records) had the highest average correlation ($r = 0.63$). Comparing this with Figure 3, these results seemed logical because the variance was mainly explained by the HTDr effect in these regions. The high proportion of variance explained by HTDr suggests that the wavenumbers are influenced by test-day factors, such as daily changes of feed, climatic conditions, or laboratory environment. Therefore, when the HTDr effect is not known (i.e., scenarios 1, 2, and 4), wavenumber predictions for this region have low accuracy. According to Socrates (2001), these regions are not very associated with main chemical information such as fat, protein, or lactose content, but these could be associated with minor components.

To our knowledge, no other authors studied the predictability of spectral wavenumbers, so comparison with the existing literature is difficult. However, Dagnachew et al. (2013a) showed that for goat milk spectra PC scores for future records could be predicted with reasonable accuracy (correlations between observed and predicted PC scores ranged between 0.48 and 0.75 for the first 7 PC). In the present study, correlations between observed and predicted PC scores for the 12 retained PC varied from 0.83 to 0.98 for the modeling data set. Correlations between observed and predicted PC scores could not be calculated for the scenarios because observed PC scores were not available as PCA was applied on modeling spectra only. The interpretation of individual spectral wavenumber correlations and variance ratio variability is complicated because milk MIR spectra represent a combination of many different molecules in milk (Soyeurt et al., 2010). Not all wavenumbers have the same contribution in the prediction of specific traits and variation in spectral wavenumbers predictions might affect MIR trait predictions differently. For instance, chemical bonds that include nitrogen molecules (e.g., N-H, C-N) are specific to protein but less interesting to predict milk fat content (Socrates, 2001). Hence, comparing MIR traits predicted on modeled MIR spectra would be relevant.

Predictions of MIR Traits

One interest of the prediction of MIR traits on the modeled spectra was to see if the accuracy did not decrease compared with the prediction of spectral

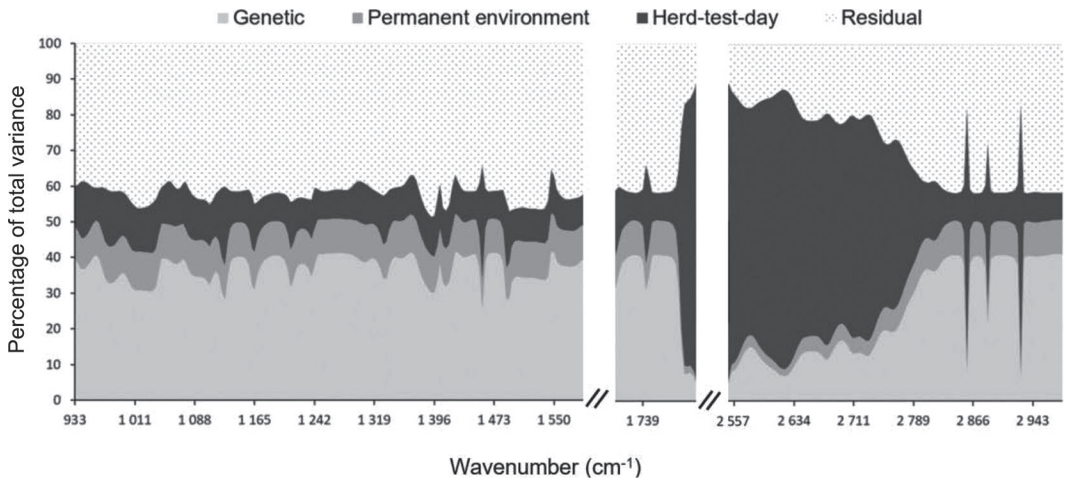

Figure 3. Percentage of total variance of spectral wavenumbers retained by the model explained by genetic, permanent environmental, herd-test-day, and residual effects.

wavenumbers and if predicted phenotype values were in an acceptable range. The left side of Table 3 presents correlations between predictions of milk fat, protein, and lactose contents from observed or modeled spectra. Correlations were relatively high for the modeling data set as they were above 0.80. Regarding the scenarios, the first one had the highest correlation values for fat and lactose content (0.63 for both traits), and scenario 3 had the highest values for protein content (0.73). Scenarios 2 and 4 had the lowest values for the 3 milk components (i.e., 0.36, 0.62, 0.46 and 0.40, 0.64, 0.32 for fat, protein, and lactose contents, respectively). Compared with fat and lactose contents, correlations for protein content showed a lower overall variation for the 4 scenarios. Globally, correlations for fat, protein, and lactose contents varied in accordance with the evolution of correlations for spectral wavenumbers in the regions 933 to 1,589 cm^{-1}, 1,704 to 1,786 cm^{-1}, and 2,777 to 2,981 cm^{-1} (Figure 5). These spectral regions are associated with molecular functional groups belonging to major milk components like lipids, proteins, or carbohydrates (Socrates, 2001; Iñón et al., 2004; Dagnachew et al., 2013a). Milk fat is mainly associated with 2 spectral regions where the carbon–hydrogen groups (C–H) and the carbonyl groups (C = O) of milk fat absorb, that is to say at 2,873 and 1,747 cm^{-1}, respectively (Socrates, 2001; Iñón et al., 2004). The region around 1,100 cm^{-1} is associated with lactose content (Picque et al., 1993).

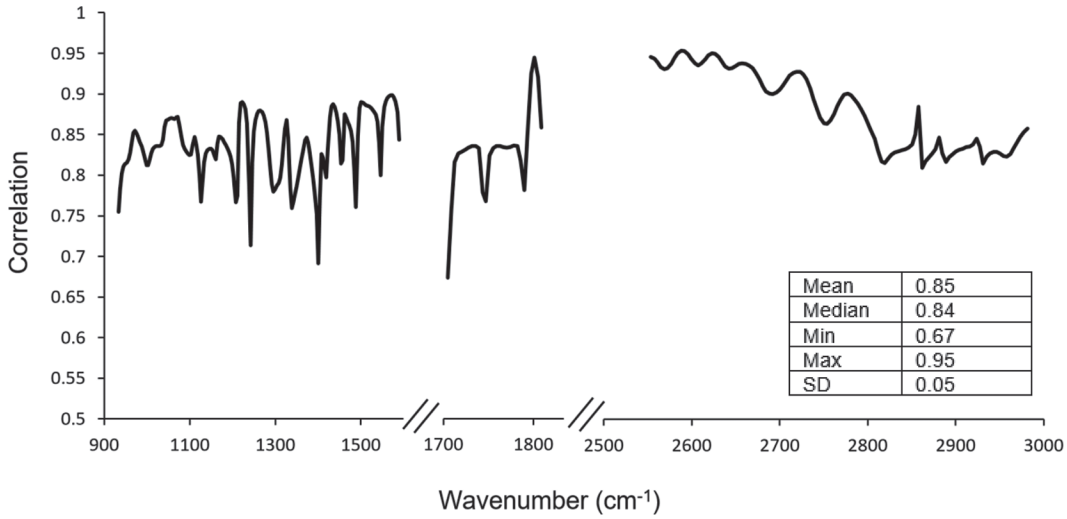

Figure 4. Correlations between observed and predicted values for the 311 spectral wavenumbers for the modeling data set. Min = minimum; Max = maximum.

Table 2. Descriptive statistics of correlations between observed and predicted values for the 311 spectral wavenumbers for the 4 scenarios

Scenario	Mean	Median	Minimum	Maximum	SD
1	0.56	0.62	0.06	0.72	0.15
2	0.37	0.37	0.00	0.61	0.13
3	0.62	0.59	0.30	0.89	0.12
4	0.36	0.38	0.05	0.63	0.14

The MIR regions located between 1,200 to 1,450 cm^{-1} and 1,500 to 1,600 cm^{-1} correspond to protein content (Sivakesava and Irudayaraj, 2002). Superior accuracy for wavenumbers and MIR traits predictions for scenario 1 and 3 were justified by the higher number of known effects in the model compared with scenarios 2 and 4. We expected that scenario 4 would produce the least accurate results given the little number of known effects included in the model. However, we noticed that scenario 4 marginally outperformed scenario 2 for some wavenumbers and for the prediction of fat and protein contents, even though HTY and HTM effects were unknown. This might partly be the consequence of the different herds and cows and the different number of observations between these 2 scenarios. Indeed, scenario 4 was composed of different cows and herds from those in the modeling set. In contrast, scenarios 1, 2, and 3 were partially connected to the modeling set and between them because they were composed of similar herds (i.e., known HTY and HTM), though they were of different size. Unfortunately, we are unable to verify this hypothesis with certainty due to the structure of the data sets.

For the 3 studied milk components, comparing the left and right parts of Table 3, correlations between traits predicted from observed spectra versus traits predicted from spectra modeled from a TDM were very similar to correlations between traits predicted from observed spectra versus traits predicted directly from a TDM. This implies that, for these traits, using prediction equations on MIR spectra predicted from a TDM did as good as modeling traits directly using a TDM. For future research, it might also be useful to consider other traits such as fine milk components that are less correlated with the major sources of variation of the spectra (Bonfatti et al., 2017).

Table 4 displays mean values and standard deviations for fat, protein, and lactose contents predicted from observed or modeled spectra and RMSE between these traits predicted from observed versus modeled spectra. For the modeling data set and the 4 scenarios, mean values predicted from modeled spectra were very similar to mean values predicted from observed spectra, but standard deviations were smaller. It shows the ability of the model to predict values in a similar range as traits predicted from observed spectra on average (i.e., close to reality), but with lower variability. In all situations, the RMSE was the highest for milk fat content, followed by protein content and then lactose content. Values for RMSE were in similar ranges compared with the standard deviation for the traits predicted from the observed spectra for the modeling set. This indicates that the error is relatively large compared with the expected variation of the observed traits in the population. The RMSE was slightly lower for the first scenario (i.e., prediction of future records) compared with the 3 other cases, in line with globally higher correlations (Table 3). Even when knowing very few information about the cow like for scenario 4 (i.e., only genetic and DIM effects were known), correlations for the 3 studied milk traits were still higher than zero and the RMSE did not increase sharply (Tables 3 and 4).

Practical Use for Herd Management

The objective of this study was to test the ability of a test-day mixed model to predict milk MIR spectra with the perspective of herd management. Today numerous traits are predicted from milk MIR spectra

Table 3. Left side: correlations between fat, protein, and lactose contents (g/dL of milk) predicted from observed spectra versus from spectra modeled from a test-day model (TDM); right side: correlations between fat, protein, and lactose contents (g/dL of milk) predicted from observed spectra versus modeled directly using a TDM[1]

	Traits predicted from observed spectra vs. from modeled spectra from TDM			Traits predicted from observed spectra vs. modeled directly from TDM		
Item	Fat	Protein	Lactose	Fat	Protein	Lactose
Modeling set	0.83	0.89	0.83	0.83	0.90	0.86
Scenario 1	0.63	0.68	0.63	0.63	0.68	0.59
Scenario 2	0.36	0.62	0.46	0.37	0.60	0.37
Scenario 3	0.53	0.73	0.46	0.53	0.72	0.46
Scenario 4	0.40	0.64	0.32	0.40	0.64	0.31

[1]Results are presented for the modeling data set and the 4 scenarios.

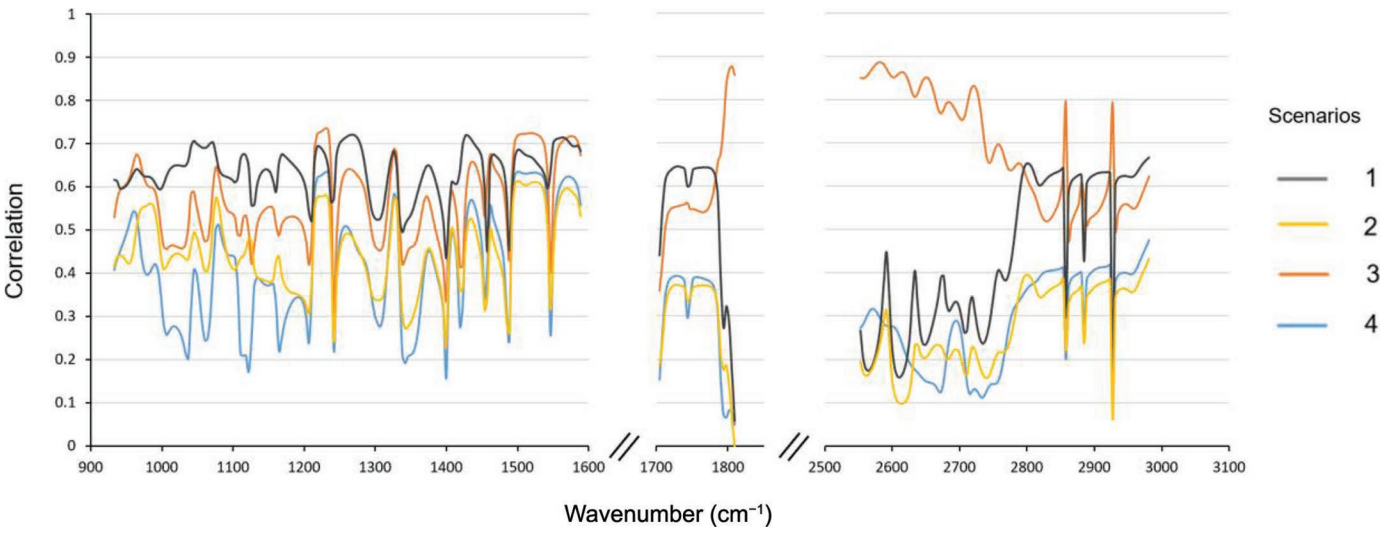

Figure 5. Correlations between observed and predicted values for the 311 spectral wavenumbers for the 4 scenarios.

(Gengler et al., 2016). One advantage of modeling the MIR spectrum compared with modeling MIR traits directly is that a limited number of models are required (i.e., one for each PC) instead of developing one model separately for each of the existing MIR traits. Then the existing calibration equations for MIR traits can be applied on the modeled spectra to predict the different phenotypes without additional calculations. Hence, it reduces the workload associated with the development of several models for the numerous MIR traits, as well as computation time and resources [e.g., there is no need to estimate variance components (REML) for each trait, which is computationally demanding]. Also, the information contained in the MIR spectrum is richer than the information in a few predicted traits and could be used as such. The information resulting from MIR spectra modeling could benefit farmers with their cow and herd management in many ways. Any unexpected variation from a usual pattern may indicate a problem. Consequently, the difference between observed and modeled (i.e., expected) spectra and resulting predicted MIR traits could be a way to detect problems such as metabolic disorders, feeding problems, or mastitis at the cow or herd level. It would help saving medical treatment costs and avoid loss of money caused by decreasing productivity or degradation of health. For example, changes in milk fat and protein ratio compared with an expected pattern can be used to detect the risk of metabolic disorders in lactating cows such as ketosis (Duffield et al., 1997), or unexpected changes in milk lactose, protein, and minerals content can be use to detect mastitis (Hamann and Krömker, 1997). In addition, MIR spectra modeling could be used for simulations through adjustments of factors in the model (e.g., to predict the results of diet or genetic changes), for prediction of missing or future records or prediction of heifer productive potential. Also, as suggested by Mayeres et al. (2004), Koivula et

Table 4. Mean (SD in parentheses) for fat, protein, and lactose contents (g/dL of milk) predicted from observed and modeled spectra and root mean square error (RMSE) between fat, protein, and lactose contents predicted from observed versus modeled spectra for the modeling data set and the 4 scenarios

	Fat			Protein			Lactose		
Item	Mean obs. spectra[1]	Mean pred. spectra[2]	RMSE	Mean obs. spectra	Mean pred. spectra	RMSE	Mean obs. spectra	Mean pred. spectra	RMSE
Modeling set	4.01 (0.68)	4.01 (0.53)	0.38	3.41 (0.38)	3.42 (0.32)	0.17	4.83 (0.17)	4.82 (0.14)	0.10
Scenario 1	4.30 (0.70)	4.22 (0.46)	0.55	3.68 (0.36)	3.67 (0.26)	0.27	4.72 (0.17)	4.75 (0.12)	0.14
Scenario 2	3.94 (0.64)	3.89 (0.43)	0.63	3.36 (0.33)	3.34 (0.28)	0.27	4.77 (0.17)	4.80 (0.11)	0.16
Scenario 3	4.00 (0.74)	3.96 (0.50)	0.64	3.35 (0.42)	3.34 (0.33)	0.29	4.84 (0.19)	4.85 (0.11)	0.17
Scenario 4	4.01 (0.71)	4.04 (0.31)	0.65	3.39 (0.40)	3.44 (0.25)	0.31	4.79 (0.18)	4.79 (0.06)	0.17

[1]Mean of the trait predicted from the observed spectra.

[2]Mean of the trait predicted from the modeled spectra.

al. (2007), and Bastin et al. (2009), studying any deviations in the solutions of the HTDr effect when running the model after each milk recording would enable the identification of herd-specific phenomena and management problems such as feeding problem or seasonal difficulties. Following further research on the topic, also to reach sufficient accuracy, MIR spectra modeling and resulting tools could be implemented in practice into official milk recording systems.

The results presented in this study showed that the model had moderate accuracy. Consequently, its use in the current state would be limited for instance for imputation of missing data or rough estimations for simulations when precise data are not necessary. However, several improvements of the studied model are possible, and needed, to use it for more precise applications such as the detection of cow or herd problems. Adding extra effects in the model such as the age of the cow or the gestation stage could be necessary, but such data are not always easily available for all cows and herds. Besides, the studied model focused only on first-lactation cows, but in a multi-lactation model, the herd effects and permanent environmental effects would be more precise as a consequence of having more individual data. Extending the model to a random regression model (e.g., using Legendre polynomials) might also improve predictions. There is also a need to explore further if capturing more spectral variation or more diverse variation would improve the accuracy, for instance using alternative selection of PC or investigating other methods for the reduction of spectral variables. Moreover, utilization of co-variance between PC in REML and BLUP though multi-trait analysis would possibly improve the accuracy. Even though PC are phenotypically orthogonal, they have genetic, permanent environmental, HTDr, and residual co-variance structures (Dagnachew et al., 2013a,b; Bonfatti et al., 2017; Belay et al., 2017). However, such multi-trait models are currently very computationally demanding on large data sets and could impede the implementation, which is a reason why we preferred single-trait models in this study. All these possible improvements need to be elaborated further, also to avoid limitations of the practical use of the model.

CONCLUSIONS

This study demonstrated the moderate ability to predict milk MIR spectra using a test-day mixed model. The prediction accuracy varied for the different spectral wavenumbers and depended on the effects known in different situations. This influenced the prediction accuracy of related MIR traits. More research is required to improve the accuracy of predictions for potential promising applications for dairy herd management.

ACKNOWLEDGMENTS

The first author acknowledges the support of the National Fund for Scientific Research (FRS-FNRS, Brussels, Belgium) through a grant scholarship. The authors acknowledge the milk laboratory Comité du Lait (Battice, Belgium) and the Walloon Breeding Association for providing spectral data. They also acknowledge for computational resources: the Plateau de Calcul et Modélisation Informatique (CAMI), partly supported by the FRS-FNRS under grant no. T.0095.19 (PDR "DEEPSELECT"), of the University of Liège, Gembloux Agro-Bio Tech, and the Consortium des Équipements de Calcul Intensif (CÉCI), also supported by the FRS-FNRS under grant no. 2.5020.11. Additional support for the work was provided by the FRS-FNRS under grant no. J.0174.18 (CDR "PREDICT 2"). The authors have not stated any conflicts of interest.

REFERENCES

Bastin, C., L. Laloux, A. Gillon, F. Miglior, H. Soyeurt, H. Hammami, C. Bertozzi, and N. Gengler. 2009. Modeling milk urea of Walloon dairy cows in management perspectives. J. Dairy Sci. 92:3529–3540. https://doi.org/10.3168/jds.2008-1904.

Belay, T. K., B. S. Dagnachew, Z. M. Kowalski, and T. Ådnøy. 2017. An attempt at predicting blood β-hydroxybutyrate from Fourier-transform mid-infrared spectra of milk using multivariate mixed models in Polish dairy cattle. J. Dairy Sci. 100:6312–6326. https://doi.org/10.3168/jds.2016-12252.

Bittante, G., and A. Cecchinato. 2013. Genetic analysis of the Fourier-transform infrared spectra of bovine milk with emphasis on individual wavelengths related to specific chemical bonds. J. Dairy Sci. 96:5991–6006. https://doi.org/10.3168/jds.2013-6583.

Bonfatti, V., G. Di Martino, and P. Carnier. 2011. Effectiveness of mid-infrared spectroscopy for the prediction of detailed protein composition and contents of protein genetic variants of individual milk of Simmental cows. J. Dairy Sci. 94:5776–5785. https://doi.org/10.3168/jds.2011-4401.

Bonfatti, V., D. Vicario, L. Degano, A. Lugo, and P. Carnier. 2017. Comparison between direct and indirect methods for exploiting Fourier transform spectral information in estimation of breeding values for fine composition and technological properties of milk. J. Dairy Sci. 100:2057–2067. https://doi.org/10.3168/jds.2016-11951.

Caccamo, M., R. F. Veerkamp, G. De Jong, M. H. Pool, R. Petriglieri, and G. Licitra. 2008. Variance components for test-day milk, fat, and protein yield, and somatic cell score for analyzing management information. J. Dairy Sci. 91:3268–3276. https://doi.org/10.3168/jds.2007-0805.

Capuano, E., J. Rademaker, H. van den Bijgaart, and S. M. van Ruth. 2014. Verification of fresh grass feeding, pasture grazing and organic farming by FTIR spectroscopy analysis of bovine milk. Food Res. Int. 60:59–65. https://doi.org/10.1016/j.foodres.2013.12.024.

Caredda, M., M. Addis, I. Ibba, R. Leardi, M. F. Scintu, G. Piredda, and G. Sanna. 2017. Building of prediction models by using Mid-Infrared spectroscopy and fatty acid profile to discriminate the geographical origin of sheep milk. Lebensm. Wiss. Technol. 75:131–136. https://doi.org/10.1016/j.lwt.2016.08.053.

Dagnachew, B. S., A. Kohler, and T. Ådnøy. 2013a. Genetic and environmental information in goat milk Fourier transform infrared

spectra. J. Dairy Sci. 96:3973–3985. https://doi.org/10.3168/jds.2012-5972.

Dagnachew, B. S., T. H. E. Meuwissen, and T. Ådnøy. 2013b. Genetic components of milk Fourier-transform infrared spectra used to predict breeding values for milk composition and quality traits in dairy goats. J. Dairy Sci. 96:5933–5942. https://doi.org/10.3168/jds.2012-6068.

De Marchi, M., M. Penasa, A. Cecchinato, M. Mele, P. Secchiari, and G. Bittante. 2011. Effectiveness of mid-infrared spectroscopy to predict fatty acid composition of Brown Swiss bovine milk. Animal 5:1653–1658. https://doi.org/10.1017/S1751731111000747.

de Roos, A. P. W., A. G. F. Harbers, and G. De Jong. 2004. Random herd curves in a test-day model for milk, fat, and protein production of dairy cattle in the Netherlands. J. Dairy Sci. 87:2693–2701. https://doi.org/10.3168/jds.S0022-0302(04)73396-2.

Duffield, T. F., D. F. Kelton, K. E. Leslie, K. D. Lissemore, and J. H. Lumsden. 1997. Use of test day milk fat and milk protein to detect subclinical ketosis in dairy cattle in Ontario. Can. Vet. J. 38:713–718.

Ferragina, A., C. Cipolat-Gotet, A. Cecchinato, and G. Bittante. 2013. The use of Fourier-transform infrared spectroscopy to predict cheese yield and nutrient recovery or whey loss traits from unprocessed bovine milk samples. J. Dairy Sci. 96:7980–7990. https://doi.org/10.3168/jds.2013-7036.

Gengler, N., H. Soyeurt, F. Dehareng, C. Bastin, F. Colinet, H. Hammami, M.-L. Vanrobays, A. Lainé, S. Vanderick, C. Grelet, A. Vanlierde, E. Froidmont, and P. Dardenne. 2016. Capitalizing on fine milk composition for breeding and management of dairy cows. J. Dairy Sci. 99:4071–4079. https://doi.org/10.3168/jds.2015-10140.

Gillon, A., S. Abras, P. Mayeres, C. Bertozzi, and N. Gengler. 2010. Adding value to test-day data by using modified best prediction method. Pages 171–178 in Proc. ICAR 37th Annu. Meet., Riga, Latvia. ICAR, Rome, Italy.

Grelet, C., C. Bastin, M. Gelé, J.-B. Davière, M. Johan, A. Werner, R. Reding, J. A. Fernandez Pierna, F. G. Colinet, P. Dardenne, N. Gengler, H. Soyeurt, and F. Dehareng. 2016. Development of Fourier transform mid-infrared calibrations to predict acetone, β-hydroxybutyrate, and citrate contents in bovine milk through a European dairy network. J. Dairy Sci. 99:4816–4825. https://doi.org/10.3168/jds.2015-10477.

Hamann, J., and V. Krömker. 1997. Potential of specific milk composition variables for cow health management. Livest. Prod. Sci. 48:201–208. https://doi.org/10.1016/S0301-6226(97)00027-4.

Hammami, H., B. Rekik, H. Soyeurt, C. Bastin, E. Bay, J. Stoll, and N. Gengler. 2009. Accessing genotype by environment interaction using within- and across-country test-day random regression sire models. J. Anim. Breed. Genet. 126:366–377. https://doi.org/10.1111/j.1439-0388.2008.00794.x.

Iñón, F. A., S. Garrigues, and M. De La Guardia. 2004. Nutritional parameters of commercially available milk samples by FTIR and chemometric techniques. Anal. Chim. Acta 513:401–412. https://doi.org/10.1016/j.aca.2004.03.014.

International Committee for Animal Recording (ICAR). 2017. Section 2 – Guidelines for Dairy Cattle Milk Recording. ICAR, Rome, Italy.

Kim, H.-Y. 2013. Statistical notes for clinical researchers: Assessing normal distribution (2) using skewness and kurtosis. Restor. Dent. Endod 38:52–54. https://doi.org/10.5395/rde.2013.38.1.52.

Koivula, M., J. I. Nousiainen, J. Nousiainen, and E. A. Mäntysaari. 2007. Use of herd solutions from a random regression test-day model for diagnostic dairy herd management. J. Dairy Sci. 90:2563–2568. https://doi.org/10.3168/jds.2006-517.

Lainé, A., C. Bastin, C. Grelet, H. Hammami, F. G. Colinet, L. M. Dale, A. Gillon, J. Vandenplas, F. Dehareng, and N. Gengler. 2017. Assessing the effect of pregnancy stage on milk composition of dairy cows using mid-infrared spectra. J. Dairy Sci. 100:2863–2876. https://doi.org/10.3168/jds.2016-11736.

Leclercq, G., N. Gengler, H. Soyeurt, and C. Bastin. 2013. Genetic variability of the mid-infrared prediction of lactoferrin content in milk for Walloon Holstein first-parity cows. Livest. Sci. 151:158–162. https://doi.org/10.1016/j.livsci.2012.11.002.

Mayeres, P., J. Stoll, J. Bormann, R. Reents, and N. Gengler. 2004. Prediction of daily milk, fat, and protein production by a random regression test-day model. J. Dairy Sci. 87:1925–1933. https://doi.org/10.3168/jds.S0022-0302(04)73351-2.

Mayeres, P., J. Stoll, R. Reents, and N. Gengler. 2002. Alternative modeling of fixed effects in test-day models to increase their usefulness for management decisions. Interbull Bull. 29:128–132.

McParland, S., G. Banos, E. Wall, M. P. Coffey, H. Soyeurt, R. F. Veerkamp, and D. P. Berry. 2011. The use of mid-infrared spectrometry to predict body energy status of Holstein cows. J. Dairy Sci. 94:3651–3661. https://doi.org/10.3168/jds.2010-3965.

Mineur, A., A. Köck, C. Grelet, N. Gengler, C. Egger-Danner, and J. Sölkner. 2017. First results in the use of milk mid-infrared spectra in the detection of lameness in Austrian dairy cows. ACS Agric. Conspec. Sci. 82:163–166.

Misztal, I. 2018. BLUPF90 Family of Programs. Accessed Jan. 2018. http://nce.ads.uga.edu/wiki/doku.php/.

Owen, A. J. 1995. Uses of derivative spectroscopy, UV-visible spectroscopy, application note, Agilent Technologies, Santa Clara, CA.

Palm, R. 1998. L'analyse en composantes principales: Principes et applications. Faculté universitaire des Sciences agronomiques de Gembloux.

Picque, D., D. Lefier, R. Grappin, and G. Corrieu. 1993. Monitoring of fermentation by infrared spectrometry. Alcoholic and lactic fermentations. Anal. Chim. Acta 279:67–72. https://doi.org/10.1016/0003-2670(93)85067-T.

R Core Team. 2017. R: A language and environment for statistical computing. R foundation for statistical computing, Vienna, Austria. Accessed Dec. 2017. https://www.R-project.org/.

Rinnan, Å., L. Nørgaard, and F. Van Den Berg. 2009. Data Preprocessing. Pages 29–50 in Infrared spectroscopy for food quality analysis and control. Academic Press, New York, NY.

Rovere, G., G. de los Campos, R. J. Tempelman, A. I. Vazquez, F. Miglior, F. Schenkel, A. Cecchinato, G. Bittante, H. Toledo-Alvarado, and A. Fleming. 2019. A landscape of the heritability of Fourier-transform infrared spectral wavelengths of milk samples by parity and lactation stage in Holstein cows. J. Dairy Sci. 102:1354–1363. https://doi.org/10.3168/jds.2018-15109.

Scampicchio, M., D. Eisenstecken, L. De Benedictis, C. Capici, D. Ballabio, T. Mimmo, P. Robatscher, L. Kerschbaumer, M. Oberhuber, A. Kaser, C. W. Huck, and S. Cesco. 2016. Multi-method approach to trace the geographical origin of alpine milk: A case study of Tyrol region. Food Anal. Methods 9:1262–1273. https://doi.org/10.1007/s12161-015-0308-2.

Shallue, C. J., J. Lee, J. Antognini, J. Sohl-Dickstein, R. Frostig, and G. E. Dahl. 2019. Measuring the effects of data parallelism on neural network training. J. Mach. Learn. Res. 20:1–49.

Sivakesava, S., and J. Irudayaraj. 2002. Rapid determination of tetracycline in milk by FT-MIR and FT-NIR spectroscopy. J. Dairy Sci. 85:487–493. https://doi.org/10.3168/jds.S0022-0302(02)74099-X.

Socrates, G. 2001. Infrared and Raman characteristic group frequencies contents: Tables and charts. 3rd ed. Wiley, Chichester, NY.

Soyeurt, H., D. Bruwier, J.-M. Romnee, N. Gengler, C. Bertozzi, D. Veselko, and P. Dardenne. 2009. Potential estimation of major mineral contents in cow milk using mid-infrared spectrometry. J. Dairy Sci. 92:2444–2454. https://doi.org/10.3168/jds.2008-1734.

Soyeurt, H., F. Dehareng, N. Gengler, S. McParland, E. Wall, D. P. Berry, M. Coffey, and P. Dardenne. 2011. Mid-infrared prediction of bovine milk fatty acids across multiple breeds, production systems, and countries. J. Dairy Sci. 94:1657–1667. https://doi.org/10.3168/jds.2010-3408.

Soyeurt, H., E. Froidmont, I. Dufrasne, D. Hailemariam, Z. Wang, C. Bertozzi, F. G. Colinet, F. Dehareng, and N. Gengler. 2019. Contribution of milk mid-infrared spectrum to improve the accuracy of test-day body weight predicted from stage, lactation number, month of test and milk yield. Livest. Sci. 227:82–89. https://doi.org/10.1016/j.livsci.2019.07.007.

Soyeurt, H., I. Misztal, and N. Gengler. 2010. Genetic variability of milk components based on mid-infrared spectral data. J. Dairy Sci. 93:1722–1728. https://doi.org/10.3168/jds.2009-2614.

Tsuruta, S., I. Misztal, and I. Strandén. 2001. Use of the preconditioned conjugate gradient algorithm as a generic solver for mixed-model equations in animal breeding applications. J. Anim. Sci. 79:1166–1172. https://doi.org/10.2527/2001.7951166x.

Van de Voort, F. R. 1992. How does material resource adequacy affect innovation project performance? A meta-analysis. J. Prod. Innov. Manage. 34:842–863. https://doi.org/10.1111/jpim.12368.

Vanlierde, A., H. Soyeurt, N. Gengler, F. G. Colinet, E. Froidmont, M. Kreuzer, F. Grandl, M. Bell, P. Lund, D. W. Olijhoek, M. Eugène, C. Martin, B. Kuhla, and F. Dehareng. 2018. 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. J. Dairy Sci. 101:7618–7624. https://doi.org/10.3168/jds.2018-14472.

Visentin, G., A. McDermott, S. McParland, D. P. Berry, O. A. Kenny, A. Brodkorb, M. A. Fenelon, and M. De Marchi. 2015. Prediction of bovine milk technological traits from mid-infrared spectroscopy analysis in dairy cows. J. Dairy Sci. 98:6620–6629. https://doi.org/10.3168/jds.2015-9323.

Wang, Q., A. Hulzebosch, and H. Bovenhuis. 2016. Genetic and environmental variation in bovine milk infrared spectra. J. Dairy Sci. 99:6793–6803. https://doi.org/10.3168/jds.2015-10488.

Wiggans, G. R., and M. E. Goddard. 1997. A computationally feasible test day model for genetic evaluation of yield traits in the United States. J. Dairy Sci. 80:1795–1800. https://doi.org/10.3168/jds.S0022-0302(97)76113-7.

Zaalberg, R. M., N. Shetty, L. Janss, and A. J. Buitenhuis. 2019. Genetic analysis of Fourier transform infrared milk spectra in Danish Holstein and Danish Jersey. J. Dairy Sci. 102:503–510. https://doi.org/10.3168/jds.2018-14464.

ORCIDS

P. Delhez https://orcid.org/0000-0002-2699-1135
F. Colinet https://orcid.org/0000-0002-5829-0907
N. Gengler https://orcid.org/0000-0002-5981-5509
H. Soyeurt https://orcid.org/0000-0001-9883-9047