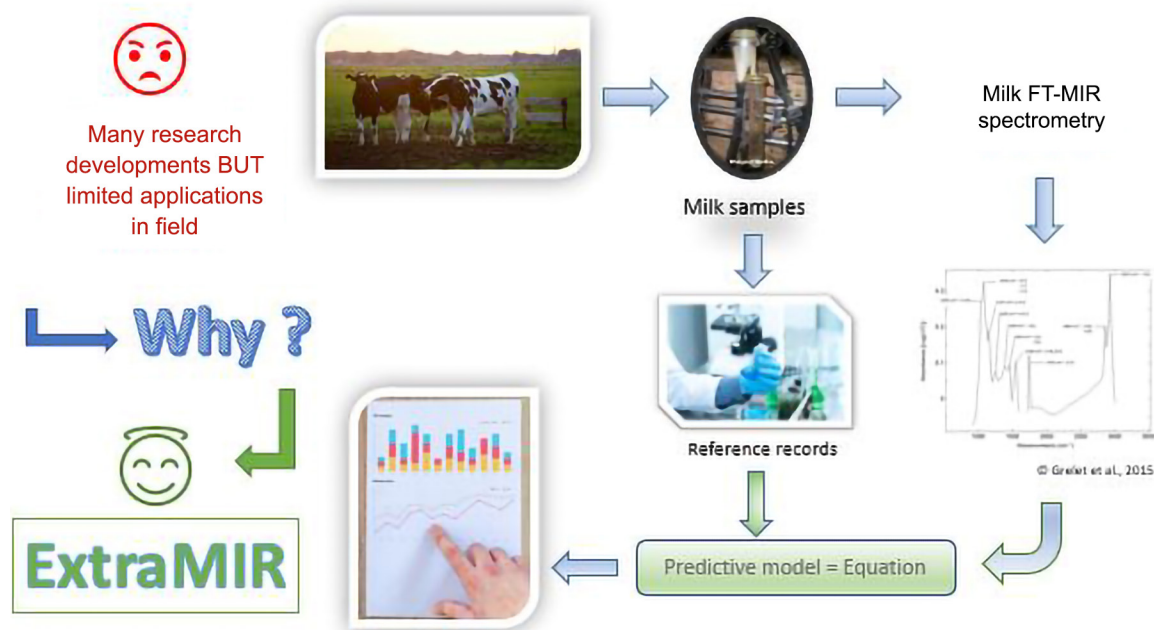


Fourier transform mid-infrared milk screening to improve milk production and processing

H. Soyeurt*

Graphical Abstract

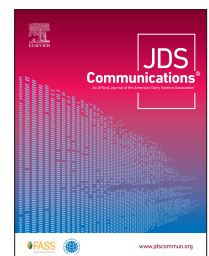


Summary

Many research developments have been done with milk Fourier transform mid-infrared (FT-MIR) spectrometry during the past 20 years, but only a few applications have been implemented in the field. ExtraMIR will try to solve the intrinsic and extrinsic constraints leading to this situation.

Highlights

- Intrinsic and extrinsic constraints explain the gap between research and the field.
- The calibration set used often has a lack of representativeness.
- There is a lack of a common validation set.
- Communication between stakeholders is too poor to favor the use of FT-MIR technology.



Fourier transform mid-infrared milk screening to improve milk production and processing

H. Soyeurt* 

Abstract: Milk mid-infrared spectrometry has been used for many years to quantify major milk compounds. Recently, much research has been conducted to extend the use of this technology to predict new, relevant phenotypes to assess the animals' welfare and the nutritional quality of milk, as well as its technological quality and environmental footprint. The transition from the research stage to field implementation is not easy, due to intrinsic and extrinsic constraints, but some developments can be considered to address these issues.

The consumption of dairy products is well anchored in the food traditions of developed countries. More than 6 billion people consume milk and dairy products worldwide (OECD and FAO, 2019). However, a relatively stable trend in dairy consumption is expected toward 2028 in Europe (37,944 t in 2022 for fresh dairy products vs. 39,942 t in 2028) and a slight decrease in the United States (22,036 t in 2022 for fresh dairy products vs. 21,471 t in 2028) (OECD and FAO, 2019). There are 2 main reasons for this. First, some consumers have a negative perception of the health aspects of consuming milk and dairy products (Zhang et al., 2021). However, milk provides 9% of dietary energy in Europe and Oceania; 19% of dietary protein supply in Europe; and 12 to 14% of dietary fat supply in Europe, Oceania, and the Americas (OECD and FAO, 2019). The second reason is that some consumers have negative perceptions about animal welfare and the environmental effect of milk production and processing in terms of carbon emissions (Adams et al., 2021). Investing in data acquisition related to these topics and their use will also have effects on farms (e.g., feed management, animal health, sustainability, profit, and so on), milk collection (e.g., detection of abnormal milk, designating milk for certain processing, and so on), and the processing itself (e.g., improvement of the nutritional and technological properties of milk, and so forth).

Fourier-transform mid-infrared (FT-MIR) spectroscopy is a rapid, nonpolluting, and cost-effective technology due to its high throughput (100 to 600 samples per hour). It is used worldwide by milk laboratories to quantify the fat and protein content in herd bulk milk samples for milk payment purposes or to predict those traits and others to assess the performance of dairy animals from representative individual milk samples. During this analysis, a mid-infrared (MIR) beam is passed through the milk sample to measure the quantity of infrared light absorbed by the sample at different frequencies, ranging from $4,000\text{ cm}^{-1}$ to 400 cm^{-1} , which are related to the vibrations of specific chemical bonds in milk (Figure 1). The obtained spectral data contain many features that are not directly informative for a user. Therefore, there is a need to extract the most relevant information—based on what we want to predict or classify—by using a calibration equation using reference values of the desired trait. Those references can be measured in milk, sometimes in blood, or these can be related to a veterinarian's

diagnosis or estimated from respiration chambers. The value of this equation is that it can be easily applied to new samples that do not have reference measurements. This means that predictors provided by the FT-MIR analysis are mainly derived from a unique source of information, the milk FT-MIR spectrum, even if some also include other information related to animal characteristics. Therefore, if we invest in the storage of this spectral information and its corresponding quality control, it is technically very easy to predict a large number of phenotypes without increasing the analytical cost (i.e., no new sampling or spectrometric analysis). Moreover, by recording this information, it would be possible to quantify new traits from the current and past spectral records. This is of interest, especially to provide breeding values faster for animal selection, but also for herd management purposes, as it offers the possibility to study the sources of variation of this new trait on a large amount of data. This is also relevant for the dairy industry to assess the stability of the milk composition in herds to detect potential abnormal milk samples. Moreover, knowing this variability can also be an opportunity for the dairy industry to develop specific products or apply marketing strategies to improve, for instance, consumers' perceptions about the consumption of milk and its derivatives.

Many prediction equations have been developed by the scientific community. With increased consumer demand for healthier food, it could be beneficial to highlight the contents of other bioactive molecules in milk by using the FT-MIR predictions of milk fatty acids, protein fractions (Franzoi et al., 2019), minerals (Christophe et al., 2021), or lactoferrin (Soyeurt et al., 2020). Fourier transform mid-infrared spectra are also useful for assessing the technological properties of milk (Bonfatti et al., 2016). Moreover, whereas milk is an important source of nutritive elements for humans, its fine composition—or, more specifically, composition changes—is important to know, as it mirrors the metabolic and health status of the animal. This explains why some indicators related to metabolism and animal health, such as energy balance or intake (Ho et al., 2020), BW (Tedde et al., 2021a), DMI (Tedde et al., 2021b), acetonemia (Grelet et al., 2016), pregnancy status (Delhez et al., 2020), SARA (Mensching et al., 2021), fertility (Ho et al., 2019), lameness (Bonfatti et al., 2020), and so on, can be derived from the milk FT-MIR spectrum. Another important topic is the environmental footprint of milk production. For example, equations exist

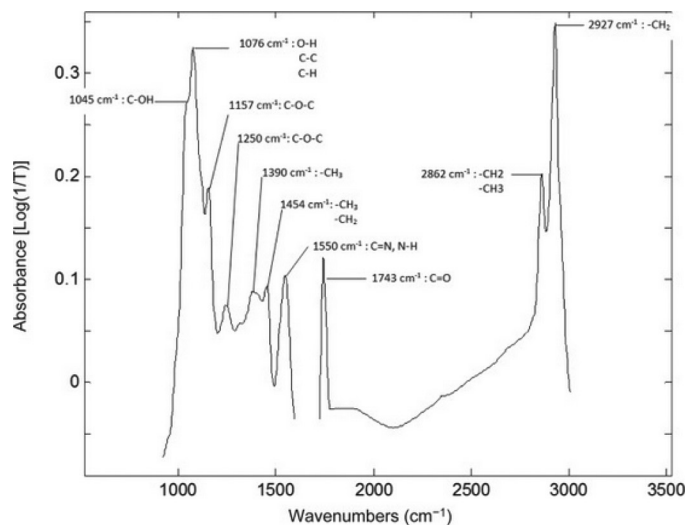


Figure 1. Milk mid-infrared spectrum (Grelet et al., 2015). T = transmittance.

to allow for the quantification of methane eructed by dairy cows (Vanlierde et al., 2016) or to assess their nitrogen-use efficiency (Grelet et al., 2020). FT-MIR spectroscopy can also be used to detect abnormal milk, as proposed by Hansen and Holroyd (2019), or to predict milk color (McDermott et al., 2016). Although this review is not complete, one can easily observe that many equations exist to provide information to the farmer, the dairy industry, and the consumer about production efficiency, its environmental footprint, animal well-being, and the nutritional quality of milk and its suitability for processing. Unfortunately, many of those equations have not yet been applied in the field due to intrinsic and extrinsic constraints.

The intrinsic constraints are directly related to the development of the predictive equation. The article published by Grelet et al. (2021) details this topic well. Here, we will highlight some points for which rapid improvement could be achieved. First, as much coverage as possible of the variability in the predicted trait existing in the studied dairy cow population and its related spectral data is required to improve the robustness of the developed models. Therefore, it is important to collect milk samples from different dairy cow populations at different moments, and receiving different diets, to achieve this objective. The design information related to the calibration set is often not given by the equation providers, who prefer to mention usual descriptive statistics, such as the mean and standard deviation. This is very problematic if we want to ensure that we are not out of the reference range when predicting the desired trait. This issue could be easily solved by fixing the parameters that need to be known (number of farms, country, diet, and so on). Moreover, detailed knowledge of the reference method used to obtain the measurements included in the calibration set is also necessary. The use of 2 different methods could result in a prediction difference. Second, we cannot confidently extrapolate the spectral data if variability is not considered in the set. Unfortunately, nothing is currently proposed to avoid this problem. However, a simple solution exists without the need to share the data sets, which may be confidential. This consists of estimating each new sample's distance from the centroid of the calibration set

used to build the equation before the prediction. If the distance is too high, the prediction must be considered with caution, because the given estimation can be the result of spectral extrapolation. Besides knowing this information to ensure the quality of the sample, the number of samples with a high global H distance could be informative for the provider, as this will highlight the need to enlarge the variability of the calibration set. Third, a sample with a high or low distance can be the result of poor-quality spectral data. So, the standardization of the spectral data based on reference samples analyzed by different spectrometers, including the master spectrometer, is of interest. It consists of comparing the spectral absorption obtained for a reference milk sample with those obtained by the master spectrometer. Then, correction coefficients can be estimated and applied to the new spectra generated by the spectrometer. This leads to better spectral quality and, therefore, to a better quality of prediction. This standardization was initially developed for near-infrared spectrometry (Bouveresse and Masart, 1996) but has been extended to milk MIR spectra (Grelet et al., 2017). This procedure can also be used to standardize spectral data from different brands of spectrometers, making the use of equations developed on another brand of spectrometer possible (Grelet et al., 2017). However, different methods exist (Bonfatti et al., 2017; Tiplady et al., 2019), and it is important to compare them to harmonize the treatment of spectra before use and to limit potential bias related to the spectral quality. Improving the spectral quality is better than directly correcting the prediction because, for some equations, such as those for methane emissions or ruminal acidosis, there is no possibility to share reference materials between laboratories through proficiency testing for fat and protein. Another challenging issue consists in comparing the prediction performances obtained from different equations built using different calibration sets or different methodologies. Theoretically, there is no problem with using different equations if we are sure that they provide similar information when they are applied to the same spectral data. This action could be easily realized using a common set of spectral data. If the predicted value is different, it is important to be sure that this is related to the prediction model and not due to another issue linked to the spectral quality, as explained before. Then, even if we have the same results, this does not automatically mean that the prediction is accurate. Currently, validation performances are communicated by the provider of the equations, but those performances are directly related to the validation set used. Therefore, it is impossible to compare the prediction accuracy of several equations predicting the same traits using this information. So, for a trait that has international interest, there is a need to organize a platform that allows equations to be validated based on a common, independent data set.

Extrinsic constraints can also explain the gap between research and field applications of milk FT-MIR equations. The first hurdle is the access to the built predictive model. The model can be developed for specific research projects that are not in line with the current desires in the field. This could happen when those in the field are not aware of the equation development and its potential. This can be explained by the fact that equation performances and their related methodological descriptions are often only published in scientific journals, which can limit access for the target audience. Moreover, there is often not enough emphasis in those articles on the aspects of application in practice. So, this lack of communication between all stakeholders can be solved by developing an in-

terface that allows private and public researchers to communicate more effectively. This interface could also propose guidance on the interpretation of those results and their potential applications for different farming conditions. Often, equations are pre-installed by the instrument provider without the option for a user to add their own equations. In the past, the spectral data were often not easily retrievable from the instrument. However, nowadays, easier access to the spectral data allows for the prediction of new phenotypes externally from the spectrometer. This explains why more and more DHI organizations have started recording spectral data to predict additional traits based on their own equations. A second extrinsic hurdle is whether there is an incentive to develop predictions for a trait. The most prominent predictions are those related to fat and protein contents because they directly determine the milk price. However, if we want to promote milk with differentiated nutritional or technological quality, it is of interest to adapt the milk price calculation to that. Some milks are better suited for milk transformation and others for milk consumption. This could also improve consumers' perceptions, as they are often unaware of the natural variation in milk composition. For instance, in the United States, cheesemakers use a specific payment equation based on fat, protein, casein, and somatic cell count to pay more for milks that will give high cheese yield. For some other traits, such as methane emissions, the incentive could be the economical sustainability of dairy farming. So, better communication is needed between all stakeholders and should focus on what is possible, scientifically justified, and practically feasible. A third extrinsic hurdle is the frequency of data acquisition, which can limit the interest of some developed equations. Milk samples are collected from the herd bulk tank when the milk is collected. This means that we have a spectral fingerprint for the herd every 2 to 3 d. This is a high frequency, which is appropriate to screen the overall composition of the milk produced on the farm. This opens up options for the presentation of trends and benchmarking in time for the specific farm and against other farms. However, herd bulk milk is a weighted average of the milk produced by each productive animal on that farm. Therefore, this sample cannot highlight problems appearing in only a few animals in the herd. For that, we need to collect milk samples individually. This is done through milk recording every 4 to 6 wk. This frequency of data acquisition is often too low to screen animal well-being as the most interesting period to detect metabolic disorders is the beginning of lactation. Two spectra can be recorded during this period if the milk sampling is done a few days after calving, but if the milk recording is scheduled for 30 DIM, there would only be 1 spectrum (Figure 2). This means that, even if the equation is relevant at the scientific level to observe metabolic disorders, the practical environment limits its use. To further optimize herd management, we can plan to organize separate collections of milk samples, especially for animals in an early stage of lactation, or to change the sampling repartition throughout the lactation (more samples at the beginning of lactation).

This article deals with many aspects related to the analysis of individual animal milk, which falls within the domain of the International Committee for Animal Recording (ICAR). As mentioned, the development and application of new milk FT-MIR models is also of value for dairy processing. Using the milk FT-MIR information, one can establish the suitability of the milk to be transformed or assess the differentiated milk quality to enlarge the brand of naturally made dairy products. By combining individual animal

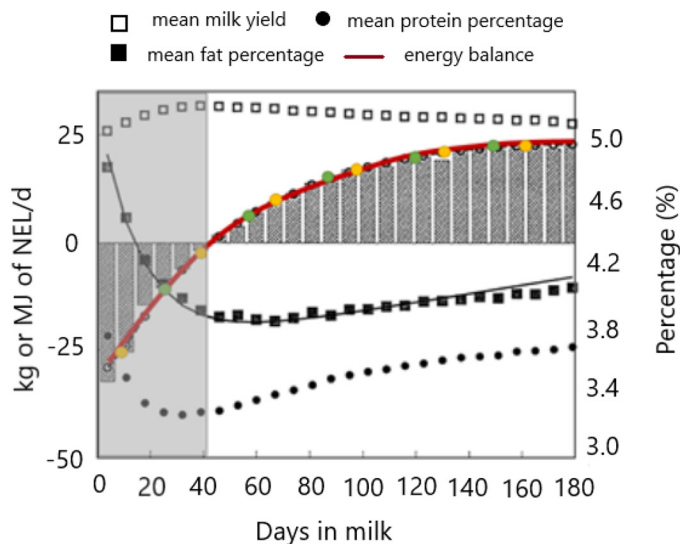


Figure 2. Energy balance, milk yield, and fat and protein percentages from calving to 180 DIM (adapted from de Vries and Veerkamp, 2000). The red line represents the evolution of the energy balance. The yellow points represent the milk recording started a few days after calving and the green points represent the milk recording started at 30 DIM.

FT-MIR information, one can evaluate the environmental footprint and animal health and welfare of the farm. This area is within the scope of the International Dairy Federation (IDF). Without doubt, there is a common interest to better exploit milk FT-MIR spectroscopy to develop specific strategies for breeding, herd management, processing, and marketing. All these aspects will also allow for the improvement of consumers' perceptions about the consumption of milk and related dairy products. By solving the different constraints mentioned previously, the gap between research and the field could narrow. Therefore, IDF and ICAR have decided to join their efforts by creating a joint ExtraMIR Action Team.

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Notes

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This study received no external funding.

This article does not contain any studies with human or animal subjects and did not require Institutional Animal Care and Use Committee or Institutional Review Board approval.

The author acknowledges each member of the “Milk Analysis” subcommittee of the International Committee for Animal Recording (ICAR) for their comments during the article’s production. Déborah Santschi and Mazen Badi from Lactanet (Montréal, Canada) are also acknowledged for their reading and comments.

The author has not stated any conflicts of interest.