J. Dairy Sci. 98:6727–6738
http://dx.doi.org/10.3168/jds.2015-9630

Visible and near-infrared bulk optical properties of raw milk

B. Aernouts,[1] R. Van Beers, R. Watté, T. Huybrechts, J. Lammertyn, and W. Saeys
KU Leuven, Department of Biosystems, MeBioS, Kasteelpark Arenberg 30, 3001 Leuven, Belgium

ABSTRACT

The implementation of optical sensor technology to monitor the milk quality on dairy farms and milk processing plants would support the early detection of altering production processes. Basic visible and near-infrared spectroscopy is already widely used to measure the composition of agricultural and food products. However, to obtain maximal performance, the design of such optical sensors should be optimized with regard to the optical properties of the samples to be measured. Therefore, the aim of this study was to determine the visible and near-infrared bulk absorption coefficient, bulk scattering coefficient, and scattering anisotropy spectra for a diverse set of raw milk samples originating from individual cow milkings, representing the milk variability present on dairy farms. Accordingly, this database of bulk optical properties can be used in future simulation studies to efficiently optimize and validate the design of an optical milk quality sensor. In a next step of the current study, the relation between the obtained bulk optical properties and milk quality properties was analyzed in detail. The bulk absorption coefficient spectra were found to mainly contain information on the water, fat, and casein content, whereas the bulk scattering coefficient spectra were found to be primarily influenced by the quantity and the size of the fat globules. Moreover, a strong positive correlation ($r \geq 0.975$) was found between the fat content in raw milk and the measured bulk scattering coefficients in the 1,300 to 1,400 nm wavelength range. Relative to the bulk scattering coefficient, the variability on the scattering anisotropy factor was found to be limited. This is because the milk scattering anisotropy is nearly independent of the fat globule and casein micelle quantity, while it is mainly determined by the size of the fat globules. As this study shows high correlations between the sample's bulk optical properties and the milk composition and fat globule size, a sensor that allows for robust separation between the absorption and scattering properties would enable accurate prediction of the raw milk quality parameters.
Key words: milk fat globule, casein micelle, visible and near-infrared spectroscopy, absorption, optical sensor design

INTRODUCTION

A precondition for increased profitability in dairy farming is an increase in both the lactation and lifetime production per cow. Therefore, more effective prevention and early treatment of all diseases, especially the so-called production diseases, are needed (Hamann and Krömker, 1997). To meet these demands, individual cow and udder health should be carefully monitored. Because milk production is a dominant factor in the metabolism of dairy cows, involving a very intensive interaction with the blood circulation, the extracted milk contains valuable information on the nutritional, metabolic, and infectious status of the cow (Hamann and Krömker, 1997; Mulligan et al., 2006; Friggens et al., 2007; Forsbäck et al., 2009; Løvendahl et al., 2010; Aernouts et al., 2011). Therefore, regular analysis of the produced milk is considered to be the most efficient way to monitor cow and udder health. Online measurement of the milk components (fat, protein, lactose, and so on) during milking twice a day would offer the potential for early detection of systemic and local alteration, thus providing a valuable input for strategic and operational management decisions (Friggens et al., 2007).

Visible (**Vis**) and near-infrared (**NIR**) spectroscopic analysis of raw milk allows for a reliable detection of the fat, protein, and lactose concentration in the laboratory (Aernouts et al., 2011). The prediction of this milk composition is mainly based on the wavelength-dependent absorption of Vis/NIR radiation by the milk constituents. The industry has recently adopted this technology and implemented it into milking systems to measure the major milk components online (Katz et al., 2011, 2003; Pinsky et al., 2013). However, despite the continuous recalibration, their accuracy and robustness is still not sufficient to support cow health management (Kaniyamattam and De Vries, 2014). This is mainly because the measured spectral signals are, next to absorp-

Received March 26, 2015.
Accepted June 4, 2015.
[1]Corresponding author: Ben.Aernouts@kuleuven.be

tion, considerably influenced by the physical properties of the milk in terms of the quantity and size of the fat globules and CN micelles. Because the refractive indices of milk fat and CN differ from that of the milk serum, the Vis/NIR radiation is forced to deviate from its straight trajectory (Tuchin, 2007). Because of these scattering processes, the traveling path of the radiation increases to an unknown extent. This complicates the prediction of the composition from measured spectra. Homogenization of the milk fat globules could reduce and standardize the Vis/NIR scattering to improve the prediction results. For example, in the early days of milk analysis, the Milko-tester (Foss Electric, Hillerød, Denmark) measured the Vis scattering after dispersion of the CN micelles and homogenization to produce a more uniform fat globule size distribution. Accordingly, the light attenuation depends mainly on the amount of fat globules and can, therefore, be used to obtain a rough estimate for the fat content (McDowell, 1968). However, because of its destructive character, high energy consumption, and significant wear and tear, the proceeding homogenization step is not desired in online analyses on farm. Alternatively, the nonlinear interference due to light scattering can be reduced with empirical methods (e.g., baseline correction, derivatives, and so on) or oversimplistic scattering models (e.g., normal, piecewise, and extended multiplicative scatter correction, path length correction method, and so on), and can be partially accounted for by the prediction models (e.g., partial least squares, support vector machines, and so on; Aernouts et al., 2011). However, these techniques only provide acceptable results for samples with absorption and scattering properties similar to those consulted in the calibration procedure (Melfsen et al., 2013). As the quantity and size of the fat globules and CN micelles for different fresh raw milk samples experience large variations, the scattering properties also vary a lot (Vangroenweghe et al., 2002; Nielsen et al., 2005; Cabassi et al., 2013; Logan et al., 2014). Consequently, it is very challenging to fully compensate for all this scattering variability with a single empirical calibration model. Therefore, more powerful and advanced techniques are needed to remove the scattering interference from the measured Vis/NIR spectra (Melfsen et al., 2012).

In Vis/NIR spectroscopy, accurate separation of the absorption and scattering properties would reduce the need for empirical scatter corrections and promote robust prediction of the sample composition (Steponavičius and Thennadil, 2009, 2011, 2013). Moreover, the pure absorption, defined as the bulk absorption coefficient $\boldsymbol{\mu_a}$ (cm^{-1}), is the probability of absorption per unit infinitesimal path length at a specific radiation wavelength and relates directly to the sample composition according to the Beer-Lambert law. The scattering, on the other hand, can be described with the bulk scattering coefficient $\boldsymbol{\mu_s}$ (cm^{-1}) and the angular scattering pattern or scattering phase function. The bulk scattering coefficient defines the probability of scattering per unit infinitesimal path length in a similar way as μ_a represents the absorption. The scattering phase function is generally too complex to reproduce and interpret and is, therefore, often represented by its mean cosine: the scattering anisotropy factor $\boldsymbol{g}$. The scattering anisotropy for biological tissues and fluids in the Vis/NIR range varies between 0 (isotropic scattering) and 1 (complete forward scattering; Tuchin, 2007). These scattering properties are determined by the physical microstructure properties of the sample (e.g., particle size distribution, particle volume concentration, material properties, and so on). For milk, this primarily relates to the quantity and size of the suspended fat globules and, to a smaller extent, the CN micelles (Bogomolov et al., 2012, 2013; Bogomolov and Melenteva, 2013; Dahm, 2013; Kucheryavskiy et al., 2014; Aernouts et al., 2015). As these properties affect the physicochemical, functional, and sensory characteristics of the raw milk and derived dairy products, they are important quality parameters (Michalski et al., 2003, 2004; Walstra et al., 2006; Cabassi et al., 2013; Schenkel et al., 2013). Moreover, the size of fat globules in milk from infected udder quarters (mastitis) is increased significantly and could, therefore, give insight into the udder health status of each individual cow and udder quarter (Erwin and Randolph, 1975; Mizuno et al., 2012). Accordingly, extraction of physical microstructure information, such as the fat globule size distribution, from isolated scattering properties would create an added value for Vis/NIR spectroscopy on raw milk (Cabassi et al., 2013; Aernouts et al., 2015).

In a single Vis/NIR spectroscopic measurement, usually reflectance or transmittance, both the effect of absorption by the chemical molecules and scattering by the physical particles are interconnected and cannot be accurately separated. Consequently, a change in the scattering properties of a measured milk sample might be misinterpreted as a change in the milk composition (Melfsen et al., 2012). On the other hand, multiple spectroscopic measurements in a slightly different configuration are not perfectly correlated and will, therefore, be influenced by absorption and scattering in a different way. The combination of such multiple measurement series with an accurate model, which mathematically describes light propagation as a function of the sample's bulk optical properties (μ_a, μ_s, and g), could provide a successful separation of the sample's absorption and scattering properties (Steponavičius and Thennadil, 2013). However, superior separation between these ab-