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Applications of NIR Spectroscopy in the Confectionary Industry

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Applications of NIR Spectroscopy in the Confectionary Industry

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25.1 INTRODUCTION

For the topic of applications of NIR spectrometry in the confectionary industry, a modest literature search using Google with the search term *NIR and confectionery* indicates the number of citations in the thousands. Furthermore, using data from Statistica, it can be gleaned that worldwide chocolate sales are 82 B $USD, while US consumption is approximately 22 B $USD and Western Europe at 39B $USD. Worldwide cocoa harvest is 4.55 million metric tons with the largest consumption being in Switzerland. This provides some perspectives on the use and potential use of analytical techniques for measuring the quality of raw and processed cocoa. NIR has broad applications in the confectionary industry segment, and some of the various applications with references will be given in this chapter. There will be a few terms that might create confusion such as *percent (%) cacao* used by some manufacturers and *percent (%) sum of cocoa solids and cocoa butter*. There are some who feel that the greater the % cacao in a product, the better it would be as a confectionary, but in an extreme case, there is a product called cocoa butter soap that approaches 100% cacao and contains no cocoa solids suitable for consumption. Note that cacao as a powder is made by cold-pressing (pressurized) unroasted cocoa beans. The result of this process is a powder retaining the natural living enzymes but with the cocoa fat (cacao butter) removed. Ingredients for chocolate: The following tables describe the common ingredients and ingredient names used for chocolate confectionary products (Tables 25.1 and 25.2).

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25.2 PARAMETERS MEASURED USING NIR

The application of NIR in the confectionery space has included the entire variety of available technologies, including filter-based instruments (tilting and discrete filters), monochromator or dispersive instruments (the most common), acousto-optic tunable filter (AOTF) systems, and Fourier transform-NIR (FT-NIR). Several manufacturers will provide basic starter calibrations, calibration services, networking, and even advanced calibrations. There are a variety of technologies and calibration approaches that are effective for measuring raw materials and processed final products.

Table 25.3 provides an example of a typical NIR instrument that has been adapted to measurements of cocoa-based products; such an instrument includes precalibrated applications, sample types, and typical data. The assays given in this table are typical for the industry.

In addition to the various lab-based NIR instruments, there are another group of instruments that have been developed to monitor parameters in real time and for potentially harsh plant process environments. One of the newer application areas that have been evolving over the last few years is the application in the detection of food adulteration. A consortium of industry, government, and

### TABLE 25.1

A List of Ingredients Present in Chocolate

<table>
<thead>
<tr>
<th>Type</th>
<th>Ingredients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dark Chocolate</td>
<td>Cacao liquor, sugar, cacao butter, lecithin, and vanilla</td>
</tr>
<tr>
<td>Milk Chocolate</td>
<td>Cacao liquor, sugar, cacao butter, milk solids, milk fat, lecithin, vanilla</td>
</tr>
<tr>
<td>White Chocolate</td>
<td>Sugar, cacao butter, milk solids, milk fat, lecithin, vanilla</td>
</tr>
</tbody>
</table>

### TABLE 25.2

Ingredient Names Common to Chocolate Confectionery Labels

<table>
<thead>
<tr>
<th>Related</th>
<th>Ingredients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cocoa Related</td>
<td>Cocoa liquor, chocolate liquor, unsweetened chocolate, cacao mass, cocoa mass, chocolate fondant, cocoa beans, cacao beans, chocolate beans, cacao seeds, cocoa seeds, chocolate seeds, cacao butter, cocoa butter, cacao oil, cocoa oil, cocoa fat, cacao fat</td>
</tr>
<tr>
<td>Dairy Related</td>
<td>Milk, cream, whole milk, condensed milk, milk crumb, dry milk powder, dry cream powder, milk solids, dry milk solids, milk fat, butter oil, butter fat</td>
</tr>
<tr>
<td>Soybean Related</td>
<td>Soy lecithin, lecithin, soya lecithin</td>
</tr>
<tr>
<td>Vanilla Bean Related</td>
<td>Vanilla bean, real vanilla, ground vanilla beans, whole vanilla beans, vanilla bean extract</td>
</tr>
</tbody>
</table>

### TABLE 25.3

Analysis of Chocolate and Cocoa Parameters Using NIR

<table>
<thead>
<tr>
<th>Constituent or Parameter</th>
<th>Measured Range (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Moisture</td>
<td>0.2%–1.8%</td>
</tr>
<tr>
<td>Dry matter</td>
<td>10.2%–52.8%</td>
</tr>
<tr>
<td>Fat</td>
<td>0.1%–18.2%; 7.5%–46.0%; 27.3%–90.7%</td>
</tr>
<tr>
<td>Solid fat at 20°C</td>
<td>48.0%–72.2%</td>
</tr>
<tr>
<td>Protein</td>
<td>2.4%–4.6%; 2.0%–4.5%</td>
</tr>
<tr>
<td>Lactose</td>
<td>0.4%–18.1%</td>
</tr>
<tr>
<td>Sucrose</td>
<td>11.5%–53.3%</td>
</tr>
<tr>
<td>Theobromines (3,7-dimethyl-1H-purine-2,6-dione)</td>
<td>1.056%–4.246 mg kg⁻¹</td>
</tr>
</tbody>
</table>
instrument company scientists published a paper on the detection of the adulteration of skim milk powder by melamine resulting from one of the first incidents of adulteration (Moros et al. 2007). For additional information on the topic of detection and analysis of food fraud and adulterants analysis, refer to Ellis et al. (2015).

25.3 NIR FOR QUANTITATIVE CONFECTIONERY ANALYSIS

In an early research report, near-infrared (NIR) spectroscopy was described as a general method for measuring a variety of food types based on the absorption of electromagnetic radiation in the wavelength range of 780–2500 nm (Osborne 2006). The NIR method is described as measuring overlapping absorption bands primarily composed of overtones and combinations of fundamental vibrational modes. The main molecular interactions involve O–H, C–H, and N–H. The measurement of the NIR spectrum, when combined with a variety of regression methods, where the reference chemical measurements are mathematically regressed against the NIR spectra, provides a method requiring from 15 to 90 s for measuring primarily moisture, protein, fat, and carbohydrate constituents in ground samples. NIR when applied to chocolate liquor or ground cocoa beans or cocoa powder provides a rapid analysis quality tool for the chocolate industry.

25.3.1 CHOCOLATE QUANTITATIVE ANALYSIS

Calibration equations for analysis of sucrose, lactose, fat, and moisture in chocolate were computed using Fourier transform near-infrared (FT-NIR) spectra (Tarkošová and Čopíková 2000). These spectra were also used for estimating rheological properties as viscosity and yield of chocolate. The NIR-predicted results were compared with the standard reference techniques for calibration and validation. The spectra of 96 chocolate samples were measured over a spectral range of 910–2500 nm using an FT-NIR Nicolet Avatar 360N spectrometer and Up diffuse reflection infrared Fourier transform (UpDRIFT) spectroscopy accessory. Mathematical preprocessing consisted of either first or second derivative was combined with a partial least squares (PLS) calibration algorithm. The models were validated using a cross-validation method. For the work, it was determined that fat, lactose, and sucrose could be predicted with suitable accuracy. However, the predictions for moisture, viscosity, and yield were not considered accurate enough at this time. Moisture is a difficult constituent to calibrate unless based on Karl Fischer moisture reference values since oven volatiles consist of many different chemical constituents. The NIR spectra are able to measure water quite accurately if the sample reference values are accurate for water content while spectra are measured.

Artificial neural networks (ANNs) have been combined with diffuse reflectance near-infrared Fourier transform spectroscopy (DRIFTS) for measuring nutritional parameters in chocolate (Moros et al. 2007). The reference methods to obtain this information are time consuming and laborious. For this study, 36 chocolate samples were analyzed for the main nutritional parameters in chocolate, such as fat, proteins, carbohydrates, cocoa content, and energetic value. For the NIR analysis, triplicate measurements of each sample were made. After spectra were collected, cluster hierarchical analysis (CHA) was used to select both calibration and validation sets. The calibration set comprised a limited set of 19 with a validation data set of 17 unique samples. ANNs were selected as a spectral data calibration method for developing a predictive model for the nutritional parameters, based on modeling the NIR spectra compared to the reference laboratory data. Results of the calibration work were reported as the root-mean-square error of prediction (RMSEP). The resulted prediction results obtained for carbohydrates, fat, energetic value, and cocoa were 1.0% (w/w), 1.0% (w/w), 50 kJ (100 g)−1, and 1.4%, respectively. The mean difference (d_x,y) and standard deviation of mean differences (s_x,y) of the carbohydrates, fat, protein content, energetic value, and cocoa content were 0.9% and 2.4% (w/w), 0.2% and 1.0% (w/w), 9.1 and 50 kJ (100 g)−1, and −0.5% and 1.4%, respectively. The maximum relative error for the prediction (QC) of any of these parameters for a new sample did not exceed 5.2%. Of course, the limited number of samples did not yield conclusive results but indicated some significant potential for using NIR to predict complex parameters in chocolate.
Near-infrared spectroscopy (NIRS) was evaluated as a rapid analytical method for the determination of sucrose content in chocolate mass (da Costa Filho 2009). A variety of chocolate mass types and recipes, with a wide range of composition, were used to develop a predictive model for sucrose composition. The more diverse sample set was purposed to provide improved model performance and compute a single comprehensive calibration. Calibration methods used included classical multiple linear regression (MLR) and PLS. GA-MLR models were developed using a variable selection method based on the regression coefficient of the PLS regression vector and by applying a genetic algorithm (GA). High correlation coefficients ($r$) resulted for calibrations as 0.998, 0.997, and 0.998 for PLS, MLR, and the GA-MLR methods, respectively, and low prediction errors were achieved. The results demonstrated that NIR is suitable as a rapid method to determine sucrose in chocolate mass for typical chocolate production.

Near-infrared (NIR) spectroscopy was reported to be a useful technique for the analysis of protein, fat, sugar, and water content in chocolate base using the spectral region of 4000–12,000 cm$^{-1}$ when combined with chemometric calibration techniques (Stohner et al. 2012).

### 25.3.2 Processed Cocoa Quantitative Analysis

A study tested the use of near-infrared (NIR) spectroscopy for routine analytical prediction of biochemical quality parameters in processed cocoa. For most producers, quality control is achieved by visual inspection and sensory testing (Krähmer et al. 2015). Chromatographic methods have not proven practical for flavor evaluation due to laborious isolation and purification steps. Therefore, a rapid and reasonably accurate method would be of great benefit to the industry. The NIR method was evaluated for cocoa quality measurements, and the following results were achieved: phenolic substances ($R^2 = 0.93$), organic acids ($R^2 = 0.88$), epicatechin ($R^2 = 0.93$), lactic acid ($R^2 = 0.87$), fermentation time ($R^2 = 0.92$), and pH value ($R^2 = 0.94$).

### 25.3.3 Cocoa Bean Quantitative Analysis

Near-infrared (NIR) reflectance spectroscopy was shown to be useful for the prediction of procyanidins in cocoa beans (*Theobroma cacao*) (Whitacre et al. 2003). Procyanidins may be associated with potential health benefits. NIR spectra were used for computing a predictive model for the quantitation of procyanidin oligomers using high-performance liquid chromatography (HPLC) as reference data. The calibration set comprised cocoa beans from different seasons, geographical environments, and fermentation levels in order to provide a wide concentration range for procyanidins compared to naturally occurring levels. The predictive results for the NIR calibrations were as $R^2 = 0.983$ with standard deviation and standard error of cross-validation ratio (SD/SECV) of 5.68. A global version of the calibration resulted in an $R^2 = 0.98$ and a SD/SECV = 6.20 across 20 FOSS NIR instruments. The NIR predictive model is able to provide a rapid method for the analysis of procyanidins in cocoa liquors for quality assurance and product manufacturing.

The comparison of spectral regions, such as near-infrared (NIR) and Fourier-transform infrared (FTIR), provides additional information for cocoa powder analysis of major constituents. In one set of experiments, spectral information was compared and then combined for calibrations using 100 cocoa powder samples over the spectral ranges of 1100–2500 and 2500–16,667 nm, representing 9090–4000 and 4000–600 cm$^{-1}$ (Veselá et al. 2007). Calibration models were created for the prediction of moisture (mean = 3.98%), fat (mean = 13.51%), and nitrogen (mean = 3.77%). The ranges for the calibration samples were as follows: moisture (1.60%–7.80%), fat (2.42%–22.00%), and nitrogen (0.88%–4.48%). For the NIR spectra, prediction results as relative root mean square error of cross-validation (RMSECV/mean) were as follows: 5.2% ($R^2 = 0.94$) for moisture, 7.0% ($R^2 = 0.96$) for fat, and 1.7% ($R^2 = 0.98$) for nitrogen. These correspond to computed RMSECV values of 0.21% for moisture, 0.95% for fat, and 0.065% for nitrogen, respectively. For FTIR, the relative (RMSECV/mean) was unacceptable for moisture, 10.4% ($R^2 = 0.94$) for fat, and 3.9% ($R^2 = 0.95$)
for nitrogen. These correspond to computed RMSECV values of 1.41% for fat and 0.15% for nitrogen, respectively. The use of data fusion by combining the NIR with FTIR spectral regions allowed more detailed studies in order to characterize frequencies in one domain based on the information of the other domain. A second derivative using NIR spectra was determined to be the best overall approach.

FT-NIR spectroscopy was evaluated for nondestructive evaluation of cocoa bean quality. The feasibility study for using NIR for analysis consisted of developing calibration models for fermentation index, total polyphenol content, and pH (Sunoj et al. 2016). The cocoa pod samples were pretreated by storage for 0, 7, 14, and 21 days in order to test the effect on these quality parameter measurements. The set of test beans was then fermented using the heap method. For the test samples, the fermentation index range was 0.535–1.242 and the total polyphenol content ranged from 6.48 to 15.58 mg g⁻¹, with the sample pH ranging from 4.26 to 6.13. All test samples were measured over the spectral range of 12,500–3600 cm⁻¹ (800–2778 nm). Traditional quality analysis results were compared to the NIR spectra using PLS regression. Spectra were preprocessed using vector normalization, multiplicative scatter correction (MSC), and first-derivative (1D) techniques. The calibration model results were as follows: for fermentation index and total polyphenols, the coefficient of determination as $R^2$ was greater than or equal to 0.80 and pH results as $R^2<0.80$. The proposed method was quite rapid for all constituent analysis at less than 1 min total analysis time. Conventional laboratory methods require $\approx 28$ h. The conclusion was that FT-NIR spectroscopy produced rapid and accurate quality attributes of fermenting cocoa and could possibly be employed to similar food products.

Cocoa bean quality and value are often associated with the total fat content in the beans. For this reason, Fourier transform near-infrared (FT-NIR) spectroscopy was tested for total fat analysis in beans in order to evaluate its use as a rapid and accurate analysis method (Teye and Huang 2015). A unique set of calibration approaches was tested. These included the use of efficient spectra interval selection by synergy interval partial least squares (Si-PLS), support vector machine regression (SVMR), and synergy interval support vector machine regression (Si-SVMR). The calibration algorithms were compared using root-mean-square error of prediction (RMSEP) and correlation coefficient ($R_{pre}$) in the prediction set. The optimum calibration for this experiment was reported as the Si-SVMR model with an RMSEP $= 0.015\%$ and $R_{pre} = 0.9708$. This study reported that the total fat content in cocoa beans could rapidly be predicted by FT-NIR spectroscopy using the Si-SVMR calibration technique.

Near-infrared spectroscopy (NIRS) and electronic tongue (ET) technology were combined to test an analytical method for the determination of total polyphenol content (TPC) as a measure of phytochemicals in cocoa beans (Huang et al. 2014). For this experiment, 110 cocoa bean samples with different polyphenol content were measured with both NIRS and ET. Both NIR and ET were compared to the data fusion vector from NIR plus ET. The vectors from each method and the combined method were scaled using normalization and principal component analysis (PCA). Support vector machine regression (SVMR) was used to construct calibration models. Final model performance was evaluated using the correlation coefficient ($R_{pre}$), RMSEP, and bias in the prediction set. Compared with a single technique (NIRS or ET), the data fusion was superior for the determination of TPC in cocoa beans. The optimal data fusion model was achieved with $R_{pre} = 0.982$, RMSEP $= 0.900$ g/g, and a bias $= 0.013$ g/g in the prediction set. The overall results demonstrate combining NIRS and ET yielded improved prediction of TPC in cocoa beans over the individual techniques.

Near-infrared spectra and denaturing gradient gel electrophoresis (DGGE) profiles were both used to evaluate the potential for predicting the microbiological changes taking place during the fermentation of cocoa (Nielsen et al. 2008). For the experiment, cocoa bean samples were sampled at 24-h intervals, then dried, and analyzed using NIR. This represents the first study to microbiological changes during cocoa bean fermentation using DGGE as correlated to NIR using multivariate data analysis. The DGGE profiles were correlated to the NIR spectra using partial least squares regression models (PLS2). It was determined that a correlation ($r$) of 0.87 was obtained for the
bacterial-derived DGGE profiles and \( r = 0.81 \) for the yeast-derived DGGE profiles. These results were considered promising for rapid analysis of fermentation using NIR.

Near-infrared (NIR) hyperspectral imaging (HSI) over a spectral range of 1000–2500 nm (10,000–4000 cm\(^{-1}\)) was used to predict fermentation index (FI), total polyphenols (TP), and antioxidant activity (AA) of individual dry fermented cocoa beans (Caporaso et al. 2018). These beans were scanned nondestructively on a single seed basis. Cocoa bean samples for testing were selected as 10 beans from each of 17 batches. Samples were scanned as single seeds using NIR-HIS, and calibrations were developed versus reference data using PLS regression. External validation performance was determined as \( R^2 = 0.50 \) (RMSEP = 0.27) for fermentation index (FI); \( R^2 = 0.70 \) (RMSEP = 34.1 mg ferulic acid per gram) for total polyphenols (TP); and \( R^2 = 0.74 \) (RMSEP = 60.0 mmol Trolox per kilogram) for antioxidant activity (AA). It was concluded by this study that the prediction performance was suitable for screening purposes useful for food quality control applications.

Fourier transform near-infrared spectroscopy (FT-NIRS) was evaluated as an analytical technique for measuring total fungi count (TFC) (Kutsanedzie et al. 2018). TFC is used as a quality indicator for cocoa beans, as the presence of various fungi within the beans can result in a food safety problem. A solution of cocoa beans was made for multiple samples, and these were measured using FT-NIRS and correlated to the reference laboratory TFC values using a variety of chemometric calibration algorithms. These calibration methods included PLS, Si-PLS, synergy interval-genetic algorithm-PLS (Si-GAPLS), ant colony optimization – PLS (ACO-PLS), and competitive-adaptive reweighted sampling-PLS (CARS-PLS). The calibration performance test parameters included the coefficients of the prediction (\( R_p \)), the RMSEP, and the ratio of the sample range standard deviation to RMSEP (RPD). The optimum results obtained were \( 0.951 \leq R_p \leq 0.975 \) and \( 3.15 \leq RPD \leq 4.32 \), using FT-NIRS combined with the Si-GAPLS calibration algorithm. The method was reported as being suitable for the quantification of TFC in cocoa beans for quality and safety monitoring.

### 25.4 NIR FOR QUANTITATIVE CONFECTIONERY ANALYSIS

Near-infrared spectra were compared to data from a trained sensory panel for a large set of raw and roasted cocoa beans, chocolate mass, and finished chocolate (Davies et al. 1991). The sensory panel data demonstrated clear differences between samples based on geographical origin and different processing. NIR was able to discriminate raw bean data better than finished chocolate; a correlation of \( r = 0.86 \) was demonstrated between the raw bean spectra and the sensory data on finished chocolate. For discrimination of high- versus low-quality raw beans, the NIR accurately identified 64% of the low-quality samples and rejected 20% of acceptable quality samples. This was considered a positive result for feasibility for the replacement of difficult and demanding sensory analysis.

Near-infrared (NIR) spectroscopy was tested for the rapid identification of cocoa bean varieties (Teye 2016). Five cocoa bean cultivars were evaluated for discrimination using the spectral region from 10,000 to 4000 cm\(^{-1}\) (1000–2500 nm). Support vector machine (SVM) and linear discriminant analysis (LDA) algorithms were compared for discrimination capabilities. The comparison of discrimination models was based on the principal component analysis (PCA) and verified by cross-validation. The research indicated that the SVM model outperformed the LDA model. The SVM model was based on five principal components and achieved a 100% correct identification for both training and prediction sets. The five cocoa bean cultivars identified were reported as IMC 85×IMC 47, PA7×PA150, PA150×Pound7, Pd10×Pd15, and T63/967×T65/238.

Discriminant analysis was performed using FT-NIR to compare Ghana cocoa beans based on their geographical region of origin (Teye et al. 2013). For this study, NIR spectra were measured for 194 cocoa bean samples from seven cocoa-growing regions. Data analysis of the spectra included an initial PCA followed by the comparison of various algorithms for discrimination power. Four different discriminant analysis methods were compared. The compared discriminant analysis methods included K-nearest neighbor (KNN), linear discriminant analysis (LDA), support vector machine...
(SVM), and back-propagation artificial neural network (BPANN). The algorithms tested as follows: the SVM model exhibited a discrimination success rate of 100% for both the training and prediction sets with mean centering (MC). BPANN showed a discrimination rate of 99.23% for the training set and 96.88% for the prediction set. The LDA model had 96.15% and 90.63% for the training and prediction sets, respectively. KNN model had 75.01% for the training set and 72.31% for the prediction set. This work demonstrated powerful discrimination for origin of beans even from a similar geographical region.

The specifics of the fermentation process determine the cocoa flavor and taste as derived from cocoa beans. To study the effects of fermentation on the measurable chemistry of cocoa beans, a combination of analytical methods was applied. The methods evaluated included the cut test, colorimetry, fluorescence spectroscopy, near-infrared spectroscopy, and gas chromatography–mass spectrometry (GC–MS). The data obtained using these analytical techniques were evaluated using chemometric methods to examine cocoa beans sampled at different durations of fermentation and samples representing fully fermented and dried beans from all cocoa-growing regions of Ghana (Aculey et al. 2010). The results of this study were as follows: changes were observed in measured values for colorimetry (higher $a^*$ and $b^*$ values related to length of fermentation), and the volatile compound content was related to fermentation time. For example, the formation of 2-phenylethyl acetate, propionic acid, and acetoin and the breakdown of diacetyl occurred as fermentation progressed.

Cocoa bean authentication was tested using FT-NIR spectra with SVM and Si-PLS algorithms (Teye et al. 2014a). SVM was applied to discriminate between fermented cocoa beans (FC), unfermented cocoa beans (UFC), and adulterated cocoa beans having 5–40 wt/wt% content of unfermented cocoa beans (UFC); the Si-PLS model was used to quantify the UFC content in the FC samples. The SVM was found to accurately discriminate the cocoa bean samples; the identification rate obtained was 100% for both the training set and the prediction set using three principal components (PCs). The Si-PLS calibration performed with an RMSEP of 1.68% and the coefficient of correlation in prediction ($R_{pred}$) = 0.98 for % UFC in FC. It was concluded that FT-NIR spectroscopy together with the tested algorithms was useful for both identification of fermented and unfermented cocoa beans and quantification of UFC down to 5% concentration in FC.

Data fusion combining near-infrared (NIR) spectra and electronic tongue (ET) data was tested together for the classification of five cocoa bean varieties (Teye et al. 2014b). PCA was used to fuse the data vectors by normalization, and SVM was used to develop the classification model. The results indicated that either single sensor (NIR or ET) was able to classify between 83% and 93% accuracy, while the SVM and data fusion (NIR plus ET) yielded a classification accuracy of 100% using three principal components for both training and prediction tests. It is concluded that ET combined with NIR data can accurately classify cocoa bean varieties. NIR has proven itself to be a cost-effective, rapid, and accurate analytical technique when properly applied for quantitative and qualitative analyses of cocoa-related products.

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