thermo scientific

APPLICATION NOTE

No. AN51892

The Analysis of Beer Components Using FT-NIR Spectroscopy

Keywords
Beverage, QA/QC, fermentation, Antaris II, beer, FT-NIR, transflectance

Introduction

Beer is a beverage produced from cereals fermentation, usually malted barley, and is believed to be the first alcoholic beverage developed by man. A beer is any variety of alcoholic beverages produced by fermentation of starch related to, or derived from, grain or other plant sources. Because the ingredients that are used to make beer differ according to region, the characteristics (e.g., type, flavor and color) vary widely. Pure beer is typically made from water, malted barley, hops and yeast unless clearly labeled otherwise, such as wheat beer. The addition of other condiments or other sources of sugar may also occur. Because beer is composed mainly of water, the origin of the water and its characteristics has an important effect on the quality of the beer, influencing, for example, the taste. Many beer styles are influenced and determined by the characteristics of water in the region where it is produced.

Yeast is used in the fermentation process to metabolize the sugars extracted from cereals, producing many compounds, including alcohol and carbon dioxide. Beers tend to have between 4% to 5% alcohol content, although this can vary considerably depending on the style and beer. In fact, there are beers with alcohol contents from 2% to over 20%.

Beer represents a significant analytical challenge because it is a very complex sample containing a wide range of components including vitamins, amino acids, proteins and bitter acids, all imparting particular organoleptic properties to the drink. The presence and quality of certain compounds are monitored to ensure a consistent product.

Figure 1:
Antaris II MDS system

Conventionally, a separate instrument is required for the analysis of each component in beer. For example, specific gravity measurements require a hydrometer. Alcohol content and specific gravity are usually determined by reference methods like distillation and pycnometry or by analytical instruments which combine oscillation-type densimetry and refractometry. In addition to organoleptical and microbiological examination for a standard beer analysis, color and bitterness are assessed by photometry; organic acids are determined using enzymatic analyses or liquid chromatography, and higher alcohols using gas chromatography. As a result of the sample preparation required for these methods, beer analysis is both time-consuming and expensive.

Fourier transform Near-infrared (FT-NIR) spectroscopy is shown in this report to be a superior method of analysis over the traditional techniques. FT-NIR measurements were performed on a Thermo Scientific™ Antaris™ II FT-NIR Method Development Sampling (MDS) System (Figure 1). This study was performed using a Thermo Scientific™ SabIR™ fiber optic probe with a transflectance accessory for measurements. The Antaris II FT-NIR instrument can analyze multiple components in a mixture with a single spectrum, and can analyze materials directly without diluting or modifying them. These key benefits make near-infrared analysis an excellent alternative to traditional methods.

ThermoFisher SCIENTIFIC

Experimental

Near-infrared spectra were collected for 27 beer standards samples. The parameters used for data collection are presented in Table 1. The spectra were collected with Thermo Scientific™ RESULT Software. All the samples were measured without any preparation using the fiber optic probe with transflectance accessory (Figure 2). Data collection time for quantitative predictions of a single standard sample was approximately 25 seconds.

Spectroscopic Range	10,000 to 4000 cm^{-1}
Resolution	8 cm^{-1}
Co-averaged Scans	32
Background	Spectralon® reference

Table 1: Spectra collection parameters

Figure 2: Data collection from transflectance module

The universal capacity of the FT-NIR technique is based on chemometrics, and allows for a correlation between the spectra and their chemical and physical properties. A calibration model was developed using the Thermo Scientific™ TQ Analyst™ Software package for quantitative analysis. In this application, the spectra were then analyzed quantitatively for alcohol content, color, refractive index and specific density. These parameters were predicted using a single FT-NIR spectrum for each of the standards sample. All spectra were mean-centered and the pathlength type used was multiplicative signal correction (MSC).

Partial Least Squares (PLS) calibration models were developed for all quantitative analysis. Each component of this quantitative method was analyzed, using different regions of the spectra. Figure 3 shows a representative spectrum, as well as, first and second derivatives spectra used for the analysis. Table 2 summarizes the parameters used for the analysis.

Using PLS regression, the FT-NIR spectra was correlated with results from reference methods to establish a model for calculation of the beer samples.

Component	Spectral Region of Analysis	Spectral Treatment	Smoothing
Alcohol	5500 – 4000 cm^{-1}	First Derivative	None
Color	9900 – 4100 cm^{-1}	None	None
Refractive Index	7000 – 4000 cm^{-1}	First Derivative	Norris Derivative (segment 5, gap 2)
Specific Density	7162 – 4099 cm^{-1}	Second Derivative	Norris Derivative (segment 3, gap 2)

Table 2: Summary of the parameters used for the analysis of beer standards samples

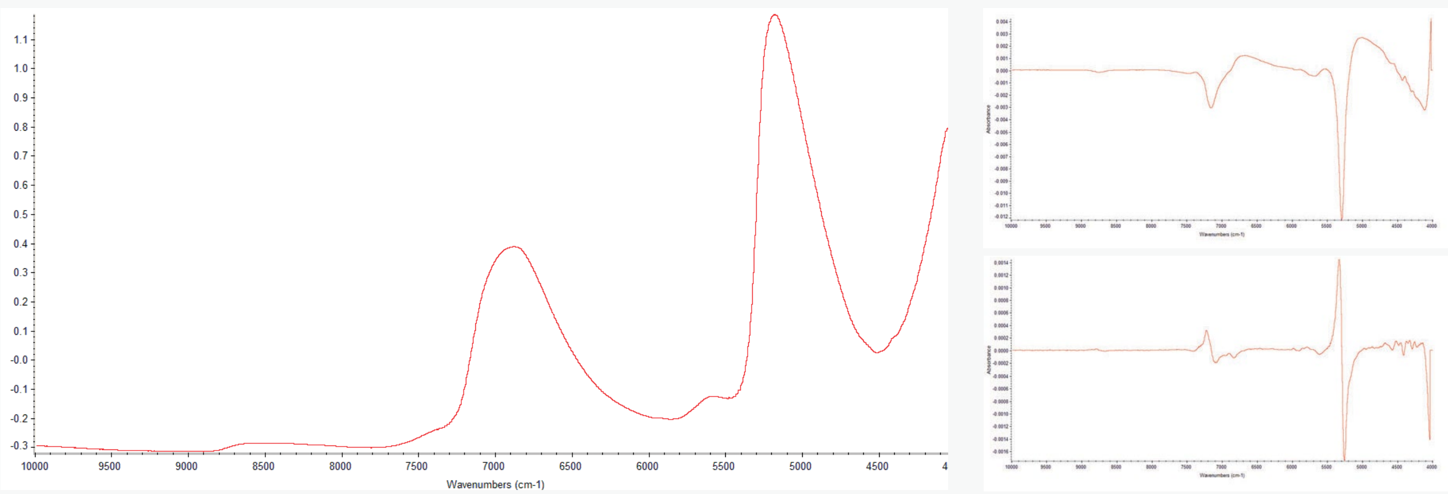

Figure 3: Representative spectrum from beer standard samples, first and second derivative of the spectrum, respectively

Quantitative analysis results

For quality control of beer, the quantitative determination of alcohol and some physical parameters were determined.

One of the quality attributes of beer that can be observed is the color. Currently, the classification of the color of beer is made during production, using a standard scale known as EBC (European Brewery Convention) where, for example, clear beer must contain less than 20 units.

The PLS model, verified through cross-validation, showed an excellent correlation between the values generated from the conventional techniques and the FT-NIR prediction. The regression lines show that there are no significant differences between the two procedures.

The samples were analyzed using a PLS method to quantify the alcohol content, color, refractive index and specific density. Figure 4 shows correlation plots between the actual value obtained with conventional techniques and the chemometric calculated values obtained with FT-NIR. We observed high correlation and low error for the four components. The method proved to be accurate and robust shown by low Root Mean Square Error of Prediction (RMSEP) and the Root Mean Square Error of Cross-Validation (RMSECV). A summary of the calibration results are presented in Table 3. The calibration data shows that it is possible to predict unknown samples accurately.

Component	Corr. Coeff.	RMSEC	RMSEP	RMSECV
Alcohol	0.99886	0.0430	0.0247	0.383
Color	0.99983	0.0315	0.0793	0.187
Refractive Index	0.99965	0.132	0.172	0.367
Specific Density	0.99619	0.188×10^{-3}	0.306×10^{-3}	0.341×10^{-3}

Table 3: Data showing calibration results

Predicted Residual Error Sum of Squares (PRESS) plots were obtained through the cross-validation metric. This diagnostic indicates the validity of the chemometric model. PRESS plots follow the expected behavior of a robust and accurate prediction chemometric model, because it shows a decrease to a minimum and then stabilization. Figure 5 shows the PRESS plots for the components measured in the beer.

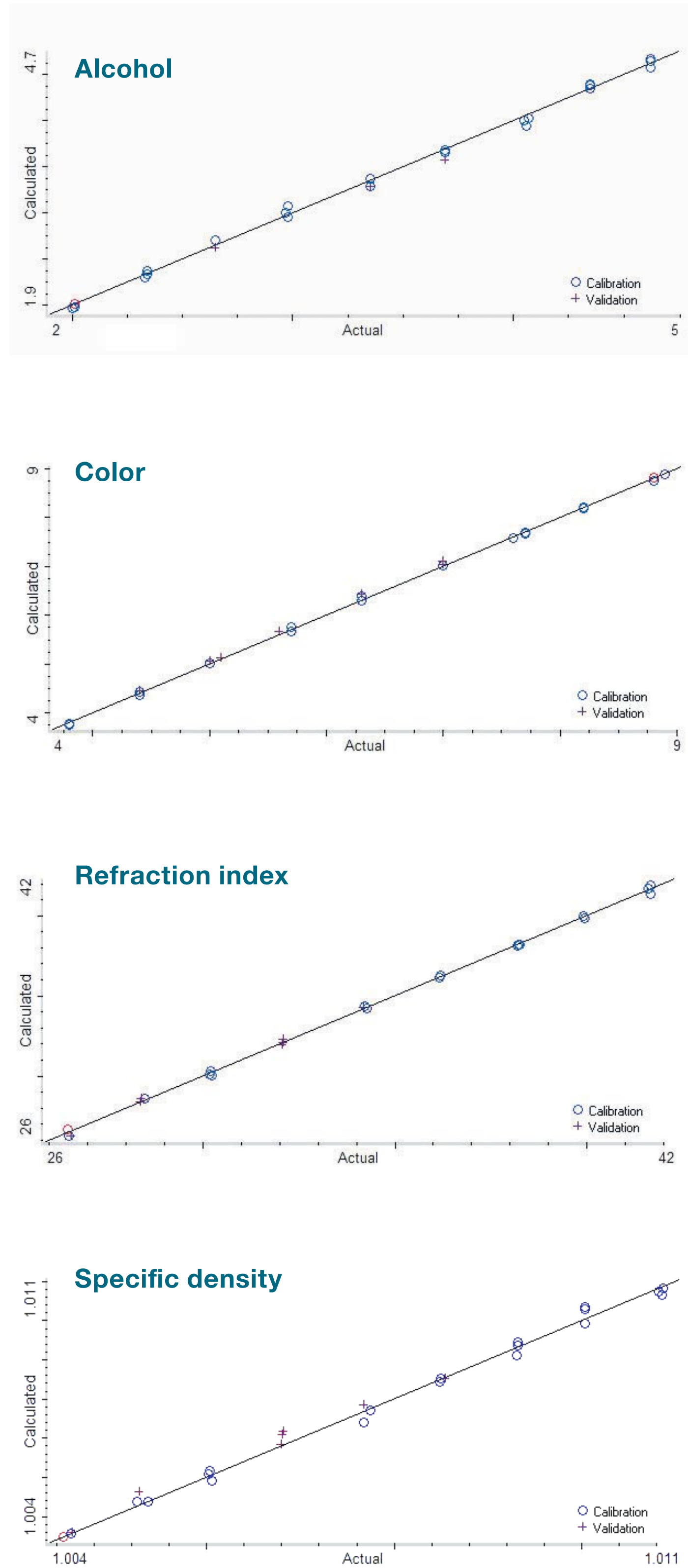

Figure 4: PLS calibration results for beer

thermo scientific

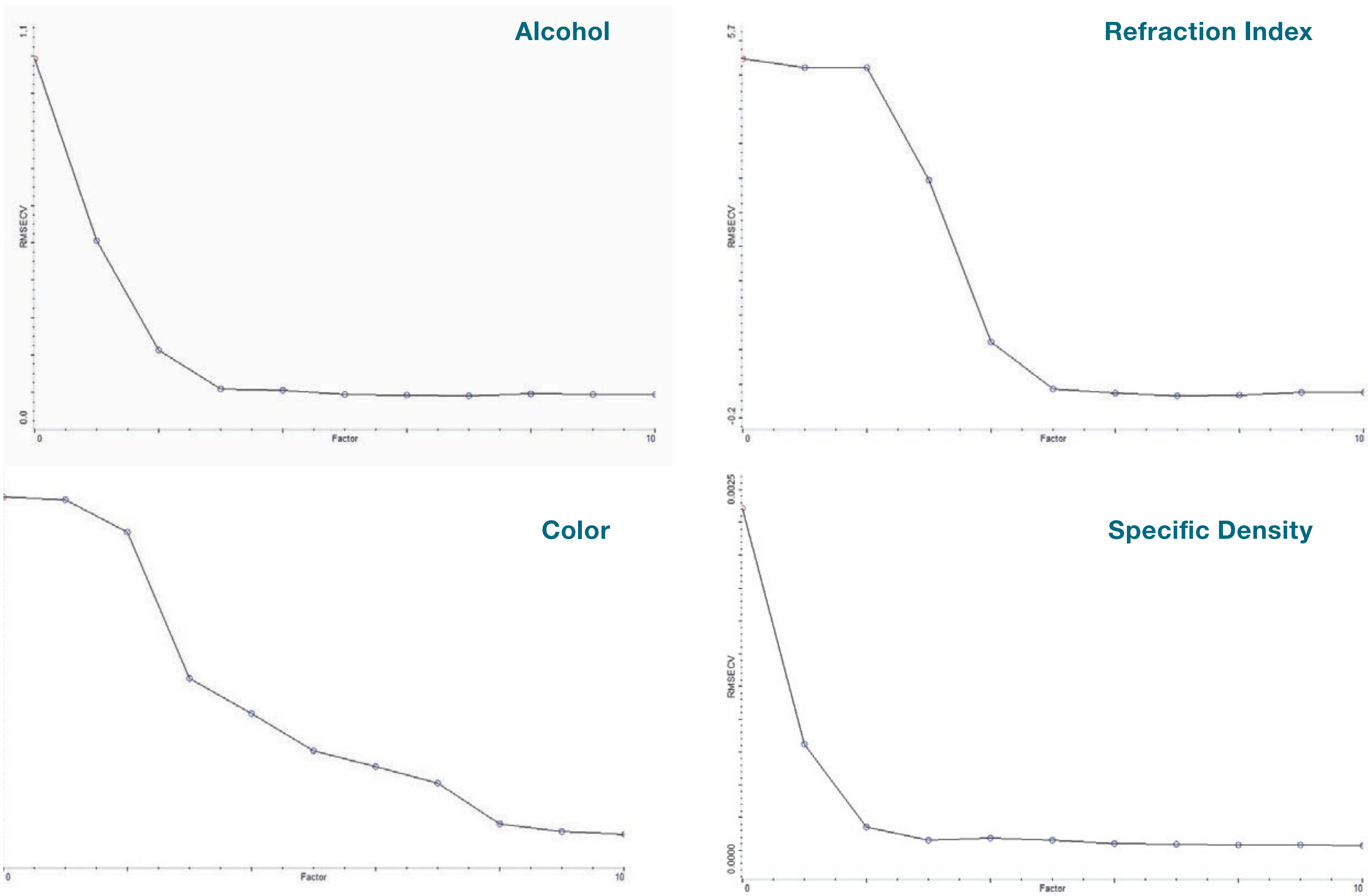

Figure 5: PRESS plots of the components measured in beer samples

Conclusion

This application demonstrates the feasibility and advantages of the FT-IR technique in beer analysis using a transflectance accessory, and also the superior speed in relation to conventional techniques. Since there is no sample preparation, it was possible to quantify multiple components simultaneously in approximately 25 seconds.

The quantitative analysis was performed on the samples using a PLS model. The results of the PLS regression models confirmed that FT-NIR spectroscopy is a suitable technique for this purpose because the calibrations are of high quality, indicating the model is appropriate and robust. Furthermore, the Antaris II FT-NIR spectrometer allows for high quality accurate measurements of multiple components in beer.

Implementation of FT-NIR methods using the Antaris II system can lead to improved efficiency, better process and quality control for the analysis of beer.

Find out more at **thermofisher.com/nir**

ThermoFisher SCIENTIFIC