APPLICATION NOTE

FT-NIR Spectroscopy

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Analysis of Properties of Wheat Using FT 9700 FT-NIR Analyzer

Introduction

Wheat has historically been a staple food source for civilizations across the world and it is still currently grown on more land area than any other commercial crop. Global production is estimated at 777 million tons for 2019/20, breaking all previous wheat production records. As a worldwide commodity, wheat is a major export for many countries and, due to an increasing global population, it is predicted that the wheat market will continue to increase accordingly.[1,2]

Harvested wheat is typically milled into flour which can then be used to make a wide range of foods, such as bread and pasta or used as raw material in feed production. Moisture and protein are key parameters for evaluating quality of a wheat sample to be used in flour milling or for setting up formulation in feed milling.

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Traditionally, these parameters are analyzed using combustion methods which can require large amounts of energy and may be time-consuming.[4] Near-infrared (NIR) spectroscopy, on the other hand, can quantify these parameters rapidly, accurately and without the need for solvents. When combined with chemometric techniques, such as partial least squares (PLS), NIR spectroscopy can provide a simple, fast and accurate method to quantifying these parameters in wheat at any stage of the production process. FT 9700™ is a new PerkinElmer FT-NIR analyzer and its' performance analysing wheat was evaluated.

Experimental

Over 490 wheat samples were collected from multiple harvests in China and Europe, allowing the natural variation within the samples to be maximized. Reference values for the analyzed parameters were collected using a PerkinElmer Inframatic 9500 NIR grain analyzer. Further moisture reference values were also collected using an oven-drying method in order to corroborate those values collected using the IM 9500 analyzer.

The samples were ground using a LM 3310 disc mill in order to minimize moisture loss within the milling process. The ground wheat samples were then scanned in replicate using multiple PerkinElmer FT 9700 analyzers, using the settings shown in Table 1.

Table 1. Scanning parameters for ground wheat samples.

Scanning Parameters	
Spectral Range	10,600 – 4,000 cm^{-1}
Resolution	16 cm^{-1}
Number of Scans	32

The number of samples used in the calibration and validation of each of the models is illustrated in Table 2. The calibrations were stabilized for natural temperature variations that may be present in the samples.

Table 2. Number of samples used in ground wheat parameter models.

Parameter	Number of Calibration Samples	Number of Validation Samples
Moisture (%)	290	66
Protein (db)	491	124

Results

The calibration plots for moisture and protein can be seen in Figures 2 and 3 respectively. The calibration (blue) and validation (red) data points are evenly distributed about the unity line, indicating a high level of agreement between the reference and predicted values for each parameter.

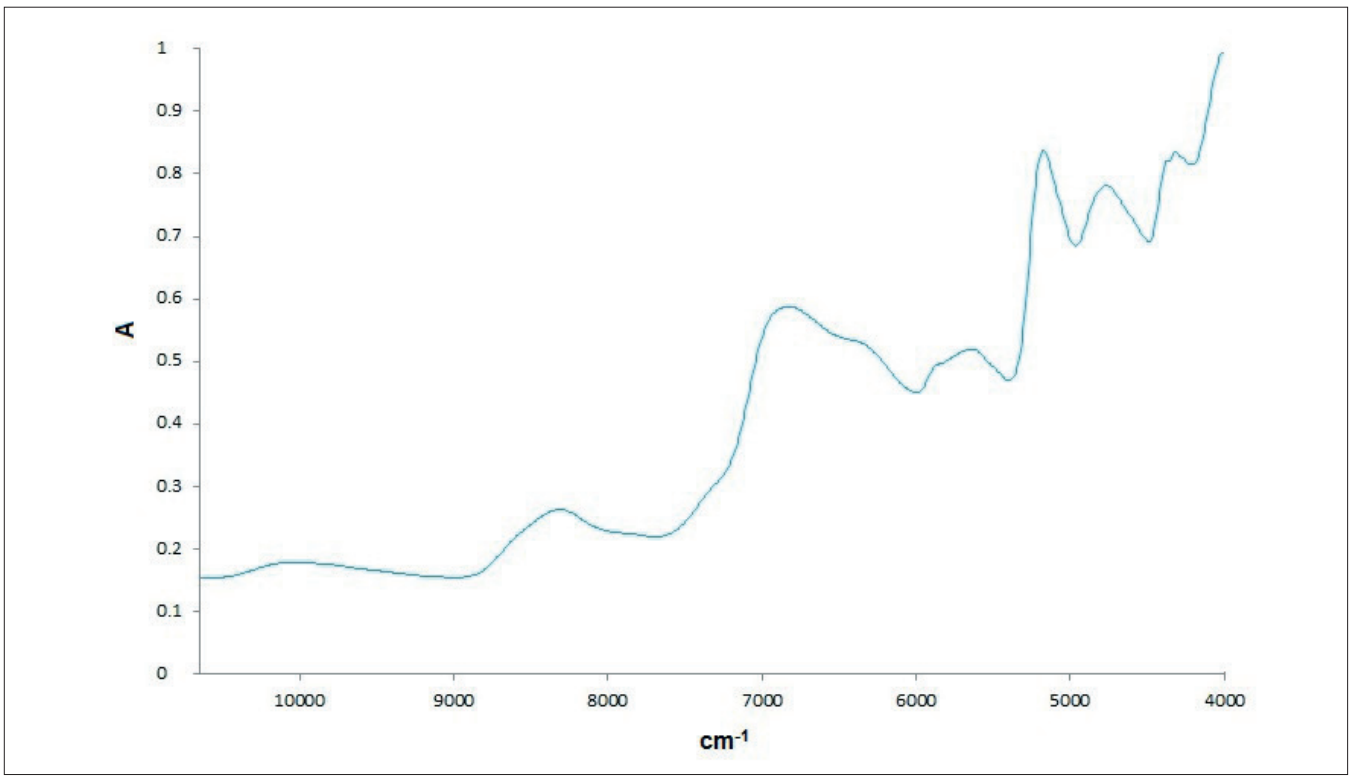

Figure 1. Example NIR spectrum of ground wheat.

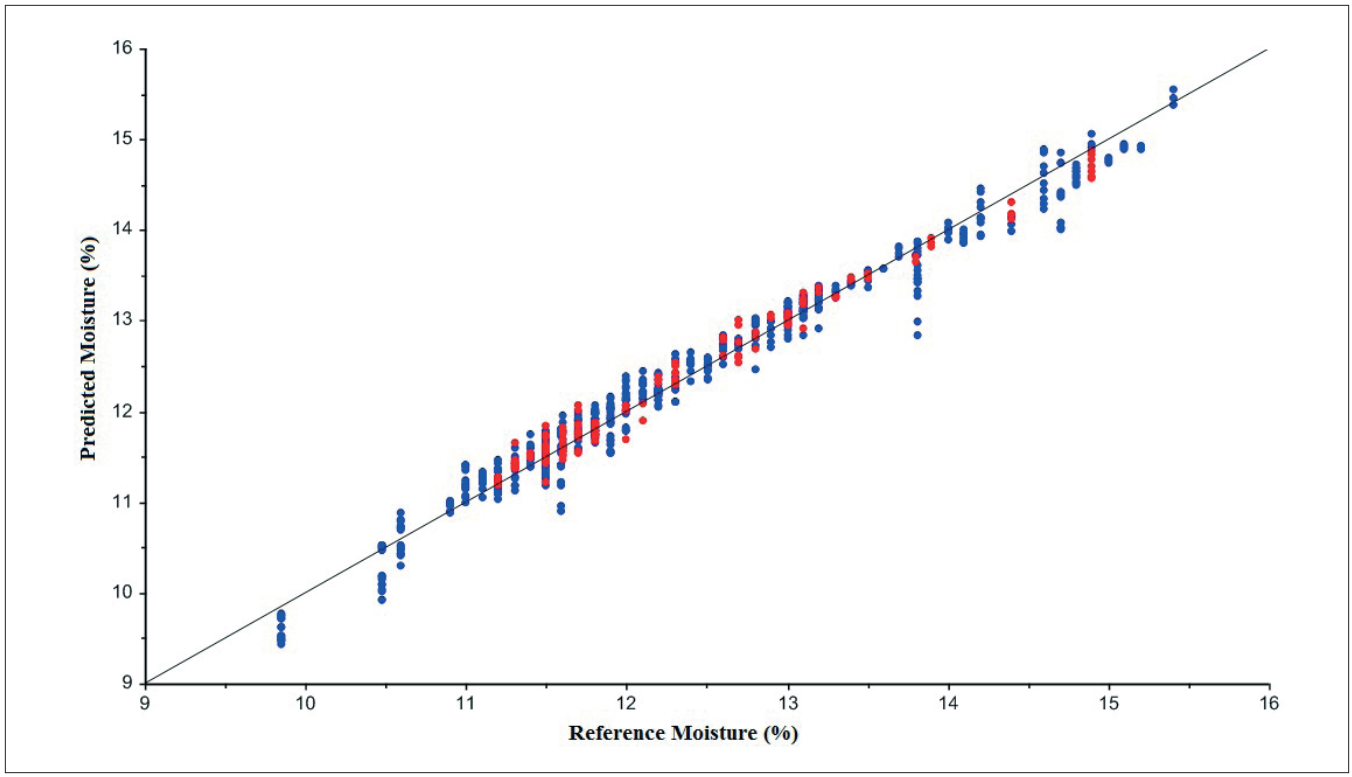

Figure 2. Correlation plot for moisture analysis of ground wheat.

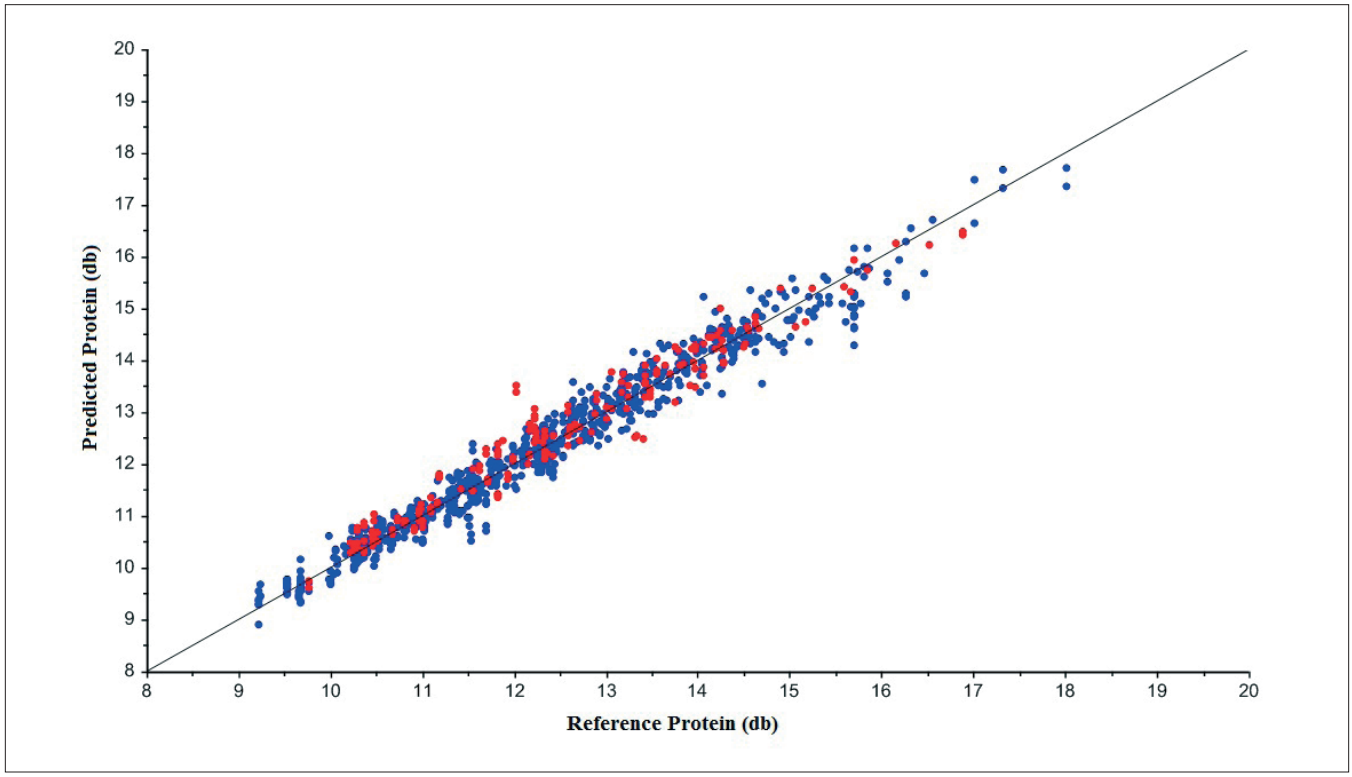

Figure 3. Correlation plot for protein analysis of ground wheat.

Table 3 illustrates the overall regression data for each of the calibration models. The R^2 value for each of the calibration models is high, further indicating the good level of correlation between the reference and predicted values. The standard error of prediction (SEP) is relatively low for each model, showing that the models have good prediction capabilities.

Table 3. Regression summary for ground wheat parameter models (where SEC is standard error of calibration and SEP is standard error of prediction).

Parameter	Range	R^2	SEC	SEP
Moisture (%)	9.85 – 15.40	0.98	0.16	0.12
Protein (db)	9.22 – 18.02	0.98	0.26	0.27

Conclusion

The results show that the FT 9700 NIR analyzer can accurately determine both the moisture and protein content in ground wheat samples. The calibration models show good correlation between the predicted and reference values. The relatively low SEP values further indicate that the models have good prediction capabilities. Additionally, the results are transferable as the spectra were collected on multiple different instruments.

Overall, the FT 9700 NIR analyzer is capable of accurately and rapidly quantifying key quality and nutritional parameters of ground wheat samples, without requiring solvents or combustion. This technique can be utilized to allow routine checks of ground wheat to be performed throughout the production process.

References

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4. *Wheat and Flour Testing Methods,* Wheat Marketing Center, Inc., 2004, pp 11-15.

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