Monitoring some quality attributes of different wheat varieties by infrared technology

Ayman Ibrahim[1*], Adrienne Csúr-Varga[2], Márton Jolánkai[2], Hani Mansour[3], Ahmed Hamed[1]

(1. *Agricultural Engineering Research Institute (AEnRI), Agricultural Research Center (ARC), Dokki, Giza, Egypt*;
2. *Crop Production Institute, Szent István University, Páter Károly utca 1, H-2100 Gödöllő, Hungary*;
3. *WRFI Dept., Agricultural and Biological Research Division, National Research Centre (NRC), Dokki, Giza, Egypt*)

Abstract: There appears to be an acceleration in the growth of non-destructive applications for monitoring and detection quality of agricultural products, especially internal quality. These technological developments have greatly increased the demand for consumers to obtain a high-quality product and safe. Near infrared (NIR) spectroscopy is one of the most important of these technologies. Accordingly, NIR spectroscopy was used to monitor and quantify the protein, gluten, moisture content, starch in some wheat varieties treated by different nitrogen fertilization rates. Partial least-squares (PLS) analysis was implemented for calibration models. The best PLS model was achieved with NIR region (1000 to 2500 nm) for protein, gluten, starch, and region from 680 to 2500 nm for moisture content. Different external validation sets were used to evaluate the accuracy of the global calibration model for protein, gluten, moisture content and starch; the coefficient of prediction (R_p^2) were 0.96, 0.98, 0.98 and 0.94, while, the ratio of the standard deviation of the reference data to the standard error of prediction (RPD) were 6.25, 6.53, 9.79 and 4.82, respectively. The precision of prediction model provided by the NIR equations confirming, that NIR technology could be a rapid, safe and precision method for wheat quality monitoring and quantification.

Keywords: Near-infrared spectroscopy, wheat quality, nitrogen fertilization, Partial least-squares (PLS)

Citation: Ibrahim, A., A. Csúr-Varga, M. Jolánkai, H. Mansour, and A. Hamed. 2018. Monitoring some quality attributes of different wheat varieties by infrared technology. Agricultural Engineering International: CIGR Journal, 20(1): 201–210.

1 Introduction

Cereal crops are known as strategic crops around the world. One of the most important crops is wheat (Triticum spp.). Not only in terms of productivity, but the quality of wheat grain has become an urgent issue as one of the most important requirements of global markets and consumer demands. As well as wheat grain and wheat products like bread, biscuit, pasta and fermented products, have numerous nutritional and health-beneficial compounds of humans where wheat grain is the main food for about one-third of the world's population (Zhao et al., 2009). Indeed, agriculture in the 21st century faces multiple challenges, the most important, expected world population to grow by over a third by 2050. In order to feed this population growth, food production must increase by 70%. Annual cereal production will need to rise to about 3 billion tons from 2.1 billion today (FAO, 2009). These growth developments in the production and consumption of wheat have greatly increased the demand for, quality and quality control in wheat grains and their derivatives. Quality of wheat grain, plays an important role in marketing of wheat. Furthermore, the end user became more demanding with regards to quality of the end product. Evidently, the priority has now gradually shifted to the quality improvement, primarily due to the increase in food diversity and market demand. Wheat is usually classified according to its variety and sub classified depending on parameters such as protein or

Received date: 2017-12-03 **Accepted date:** 2018-01-09

*** Corresponding author: A. Ibrahim,** Ph.D., Agricultural Engineering Research Institute (AEnRI), Agricultural Research Center (ARC), Dokki, Giza, Egypt. Email: aymanelgizawee@gmail.com. Tel: 01005669913, Fax: 0233356867.

gluten content. High protein and starch are important for growth and energy, where gluten, which is a complex protein made of glutenin (Gln) and gliadin (Gld), is essential for water and gas retention ability for making loaf and chapatti (Miralbes, 2008). In the light of the information was mentioned in preceding paragraph, many researchers believe that nitrogen fertilization, which is one of the most effective factors to increase yield and improve quality for wheat grains. Nitrogen, which is one of the most limiting nutrient in natural ecosystems, is required for food productivity worldwide (Giller et al., 2004). Where, the yield of wheat is a function of many factors, cultivar and nitrogen fertilization are the most important ones which influence yield, as well as the technological quality of grain (Alam et al., 2007). Grain protein content was associated mainly by the proper amount of N fertilizer application (Blandino et al., 2015). Also, the nitrogen fertilizer has a greatest influence on grain quality is achieved through its effect on grain protein concentration resulting in an increase of gliadins and glutenins (Johansson et al., 2004). Another significant factor we should also consider, the extensive use of N fertilizer unfortunately has an impact on the local environment through changes in soil microbe activity and non-agricultural plant and animal ecosystems. Nitrogen fertilizers are the largest source of N released into the atmosphere worldwide, which also represents a significant amount of the greenhouse gas emissions nitrous oxide (N_2O) and the emission of toxic ammonia into the atmosphere, also high nitrate content in plant tissues can cause toxicity problems in human's especially in infant children and also in drinking water contaminated with high NO_3, and livestock from grazing on contaminated grass as mentioned (Beman et al., 2005). Samples may also be retained for further analysis. In addition, it can also be performed by technically unskilled personnel at-line or automatically on-line. These results were confirmed by Dowell et al. (2006), where mentioned that quality characteristics of wheat whole grain, flour, dough, and bread can be measured by various qualitative and quantitative tests. There are standard or recommended measurement methods for many of these quality parameters such as those found in the Approved Methods of American Association of Cereal Chemists (AACC, 2000). These methods are generally difficult and time-consuming, and most cannot be used to rapidly measure quality characteristics and functionality. NIRS is a relatively new, promising form of technology. NIRS technique provides fast prediction values of major contents in grain products and reduces time and cost at all stages of production, storage and transport (Osborne, 2000). NIRS can measure the chemical composition of biological materials by using the diffuse reflectance or transmittance of the sample at several wavelengths as pointed (Cassells et al., 2007). Also, Burns and Ciurczak (2001) showed that Infrared Spectroscopy was commonly referred to as vibrational spectroscopy because chemical bonds had specific frequencies at which they vibrate corresponding to energy levels and when energy was absorbed, and this absorption could be measured and chemical composition could be predicted by spectrophotometers Maertens et al. (2004), In other words, NIRS can measure the concentration of components possessing different molecular structures such as protein, water, or starch (Long et al., 2008). NIRS Technology has made it possible to directly measure different constituents in the grain products. Where, the advent of NIR on-combine sensors gives the opportunity to measure the grain protein content of wheat during harvest Coefficient of Determination (R^2) was between 0.91 up to 0.94 depending on the placement of the sensor and Standard Error of Prediction (SEP) was <5.0 g g^{-1}) (Long et al. (2008). Several studies have described the NIR potential to directly measure the protein, moisture, dry weight and starch of several grains (Montes et al., 2006). By the same token, Maertens et al. (2004) built calibration models between the NIR spectra and the quality parameters by partial least-squares (PLS) algorithm, with standard error of cross-validation (SECV) around 0.57% and 0.31% for protein and moisture in wheat, respectively. Gributs and Burns 2006 reached to calibration model for moisture content estimation of wheat using wavelet transform gave high prediction accuracy with SECV of 0.096%, SEP of 0.27, and R^2 of 0.96. Ferreira et al. (2014) used near-infrared and mid-infrared (MIR) spectroscopy, with diffuse reflectance measurements, associated with multivariate calibration methods based on PLS algorithm to determine the parameters of quality, such as moisture, protein, lipid and ash content in 20 varieties of soybean. The determination coefficient (R^2) for moisture, ash, protein and lipid content were 0.72, 0.73, 0.88 and 0.81 for NIR and 0.63, 0.87, 0.91 and 0.67 for MIR, respectively, having an root mean square error of cross-validation (RMSECV) () < 2.09%. Miralbes (2008) analysed wet gluten, dry gluten, moisture, protein, and alveograph parameters (W, P, and P/L) of whole wheat using NIR transmittance spectroscopy. Modified PLS models on NIR spectra (850-1048.2 nm) were developed for each constituent or physical property. The best models were obtained for protein, moisture, wet gluten, and dry gluten with R^2 = 0.99, 0.99, 0.95, and 0.96, respectively. Lin et al. (2014) showed the results that NIR spectroscopy technique was quite useful and effective for barley GPC estimation. A relationship was established between the spectra and GPC using the LSSVR arithmetic. The calibration models are very good with high accuracy (R^2= 0.9836, SEP = 0.2276), and with robust stability. Petisco et al. (2010) studied the feasibility of visible and near-infrared (vis–NIR) spectroscopy in quantifying rapeseed quality parameters such as oil, protein and total glucosinolate contents and they reached through calibration model that R^2) and the ratio of the standard deviation of the reference data to the standard error of prediction (RPD) were 0.98 (6.5), 0.96 (4.9) and 0.99 (10.0) for oil, protein and total glucosinolate contents, respectively. The research purpose will develop a model based on the correct use of NIR calibration, for monitoring some quality attributes of different wheat varieties.

2 Materials and Methods

2.1 Samples

Samples were taken from a field experiment including three winter wheat (Triticum aestivum L.) varieties, Alföld (QA), Mv Suba (QS), and Mv Toborzó (QT), it was carried out in 2014, under zero fertilizer and three levels of nitrogen fertilization (80, 120 and 160 kg N ha^{-1}).

2.2 Spectra Acquisition

The NIR spectra acquisition for varieties of winter wheat (*Triticum aestivum* L.) was carried out using SpectraStar 2500 XL-R instrument, the spectral range 680-2500 nm and 1 nm resolution. NIR spectra were collected on approximately 30 g wheat whole grain samples with a ring cup sample cell using a standard transport module. Each spectrum was obtained from 20 scans/sample scans. The scans were averaged, transformed to log (1/R), and then stored in a computer file, forming one spectrum per each sample. After scanning, each sample was numbered for further identification. Samples were run at room temperature (23±2°C).

2.3 Calibration and validation procedure

The calibration model was performed by using the Unscrambler program V. 10.2 (CAMO Software AS, Norway). The all spectra were preprocessed by different mathematical treatments during building calibration models to obtain the best model and improve the predictability: Savitzky–Golay smoothing (SG), standard normal variate (SNV), first multiplicative scatter correction (MSC) and different combinations of these treatments were evaluated (Rinnan et al., 2009). A calibration model was developed by applying partial least squares (PLS) regression using the spectral data and reference measurement of quality parameters of wheat grain varies like protein, gluten, moisture content and starch. Therefore, the 120 samples were randomly separated into two groups: a calibration set (75% of samples) used for calibration development and a validation set (25% of samples) that were not included in the calibration development but were used to evaluate the calibration model. The accuracy of the performance calibration model was evaluated by calculating the following Key statistical indicators, coefficient of determination (R_C^2), standard error of calibration (SEC), and validation was evaluated based on the coefficient of prediction (R_P^2), standard error of cross validation (SECV), SEP, RPD and the bias (average of differences), Which the bias is a good indicator of similarity between validation samples and the calibration set. The best fitting model for prediction by quality parameters (protein, gluten, starch and moisture content) of wheat grain varieties according to its nitrogen fertilization content, was chosen based on higher R_P^2 and RPD combined with lower SEP and bias, according to Igne and Hurburgh (2010).

2.4 Reference chemical analyses

Grain samples from all wheat varieties were ground in a laboratory micro mill (TechniLab Instruments, Pequannock, N.J., Model 502) to pass 1 mm to quality analysis, all the experiments were carried out according to the Standard Methods of AACC (2000). Wheat flour samples were analyzed for protein, gluten, starch and moisture content. Protein content was determined by Kjeldehal method as stated in AACC method 46-10. A conversion factor of 5.75 was used to convert the percent of nitrogen to percent protein, and gluten content was determined using AACC standard method 38-12. A following the procedure for whole meal, in addition, starch content of grain was determined using AACC method 76-30. A damaged Starch, spectrophotometric method, where starch damage is expressed as a percentage of flour weight. While, moisture content was determined by air oven method at a temperature 105°C±5°C according to the procedure of AACC standard method 44-15A (AACC, 2000).

2.5 Statistical analysis

A randomized completely blocked design field layout design was taken. The wheat varieties were taken as replications. The treatments were the N levels of (0, 80, 120, and 160 kg ha^{-1}) for protein, gluten, moisture content and the starch which given in randomized order to minimize the effects of variation in environmental and soil conditions. The statistical package of social science (SPSS), version 20 was used in statistical analysis.

3 Results and discussion

3.1 Wheat quality parameters determined by the reference methods

Through monitoring the quality of wheat varieties studied under different levels of fertilization showed that the percentage of protein and gluten parameters increased by increasing the rate of fertilization in the varieties Alföld (QA) and Mv Suba (QS), but a low value for protein and gluten was observed at 120 kg ha^{-1}, for the value at the level 80 kg ha^{-1} in Alföld (QA) wheat variety, this is consistent with (Gauer et al., 1992; Ottman et al., 2000; Dupont and Altenbach, 2003; Johansson et al., 2004). While, it was founded that in Mv Toborzó (QT) variety, the protein and gluten values increased by increasing fertilization rates from Zero to 120 kg ha^{-1}, but recorded low values at 160 kg ha^{-1} as shown in Table 1, this confirms that extensive use of N fertilizer reduce the quality of the grain as reached (Beman et al., 2005).

Table 1 Descriptive data for some quality parameters of different Hungarian wheat varieties

Quality Parameters		Wheat varieties											
		Alföld (QA)				Mv Suba (QS)				Mv Toborzó (QT)			
		N levels, kg ha^{-1}				N levels, kg ha^{-1}				N levels, kg ha^{-1}			
		0	80	120	160	0	80	120	160	0	80	120	160
Protein, %	Min.	10.42	12.19	12.33	12.87	10.63	12.07	12.52	12.97	10.23	11.8	12.66	12.18
	Max.	12.07	13.16	12.55	13.30	11.45	12.17	13.19	13.44	10.67	12.18	12.78	12.82
	Mean	11.42	12.7	12.43	13.04	11	12.13	12.81	13.22	10.46	12.02	12.72	12.42
	SD	0.53	0.41	0.07	0.16	0.33	0.03	0.26	0.19	0.18	0.14	0.04	0.26
	CV	0.046	0.032	0.006	0.012	0.003	0.002	0.002	0.014	0.017	0.012	0.003	0.021
Gluten, %	Min.	23.2	28.5	28.8	31.3	27.95	29.5	30	32.35	21.8	26.95	29.95	29.55
	Max.	24.42	32.36	30.65	31.82	30.20	30.30	32.46	34.37	24.67	28.25	31.31	29.95
	Mean	23.85	30.19	29.72	31.53	29.25	29.82	31.12	33.08	23.21	27.76	30.54	29.76
	SD	0.48	1.60	0.75	0.18	1.04	0.30	1.00	0.84	1.22	0.52	0.51	0.12
	CV	0.02	0.053	0.025	0.0057	0.036	0.01	0.032	0.025	0.053	0.019	0.017	0.004
M.C., %	Min.	9.5	9.33	9.87	9.57	9.27	9.37	9.77	9.7	10.17	10.17	10.5	10.4
	Max.	9.65	9.49	10.05	9.82	9.68	9.70	9.87	9.95	10.34	10.31	10.61	10.48
	Mean	9.59	9.4	9.96	9.71	9.5	9.56	9.82	9.86	10.27	10.23	10.55	10.44
	SD	0.05	0.05	0.06	0.09	0.17	0.13	0.03	0.09	0.06	0.04	0.03	0.03
	CV	0.0052	0.0053	0.006	0.009	0.018	0.014	0.003	0.009	0.006	0.004	0.003	0.003
Starch, %	Min.	64.5	63.7	63.2	63.3	64.9	64.2	63	63	66.1	64.8	63.7	64
	Max.	65.56	64.94	63.64	63.92	65.76	64.95	64.05	63.44	66.63	65.43	64.25	64.95
	Mean	65.09	64.22	63.4	63.63	65.41	64.61	63.62	63.26	66.37	65.12	64	64.51
	SD	0.34	0.38	0.16	0.20	0.28	0.23	0.35	0.15	0.18	0.19	0.18	0.28
	CV	0.005	0.006	0.003	0.0031	0.0043	0.0036	0.0055	0.0024	0.0027	0.0029	0.0028	0.0043

Note: Min.: minimum value, Max.: maximum value, SD: standard deviation, CV: coefficient of variation, M.C.: moisture content.

By the same token, the moisture content "M.C." (%) and starch quality parameters, were affected by different fertilization rates, where the results obtained for the moisture content of both Alföld (QA and Mv Toborzó (QT wheat varieties were shown that, there was no effect on the increase of "M.C." (%) at 80 kg ha^{-1} level in relative to the control level. While, the value of M.C. (%) increased by 3.86% and 1.25% for Alföld (QA) variety also 2.72% and 1.66% for Mv Toborzó (QT) variety at level 120 and 160 kg ha^{-1}, respectively. Finally, Table 1 shows that by increasing nitrogen fertilization rates, the starch content of wheat grains has been decreasing for all varieties. ANOVA analysis indicated that N levels (kg ha^{-1}) at different wheat varieties have a significant ($p < 0.05$) effect on protein, gluten, moisture content, and the starch as shown in Table 2. Data analysis showed that there was a highly significant difference on the mean of all the treatments.

Table 2 Analysis of variance (ANOVA) for the effect of N levels (kg ha^{-1}) on Protein, Gluten, Moisture content and starch of three different wheat varieties

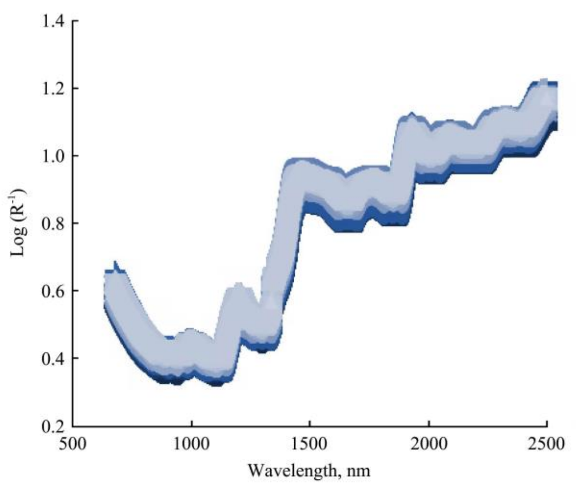
Source	Type II Sum of Squares	df	Mean Square	F	Sig.
Quality Parameter (1)	Protein content, %				
Corrected Model	72.203	5	14.441	120.872	0.000
Intercept	17856.896	1	17856.896	149467.251	0.000
block	5.419	2	2.709	22.679	0.000
treat	66.784	3	22.261	186.333	0.000
Error	13.620	114	0.119		
Total	17942.719	120			
Quality Parameter (2)	Gluten content, %				
Corrected Model	811.521	5	162.304	88.959	0.000
Intercept	101985.940	1	101985.940	55898.525	0.000
block	186.554	2	93.277	51.125	0.000
treat	624.967	3	208.322	114.182	0.000
Error	207.991	114	1.824		
Total	103005.452	120			
Quality Parameter (3)	Moisture content, %				
Corrected Model	15.788	5	3.158	313.714	0.000
Intercept	11778.234	1	11778.234	1170191.509	0.000
block	12.929	2	6.465	642.283	0.000
treat	2.859	3	0.953	94.668	0.000
Error	1.147	114	0.010		
Total	11795.170	120			
Quality Parameter (4)	Starch content, %				
Corrected Model	92.844	5	18.569	200.437	0.000
Intercept	498233.328	1	498233.328	5378065.321	0.000
block	19.458	2	9.729	105.018	0.000
treat	73.386	3	24.462	264.050	0.000
Error	10.561	114	0.093		
Total	498336.733	120			

Note: Sig. 0.000 means $p<0.05$.

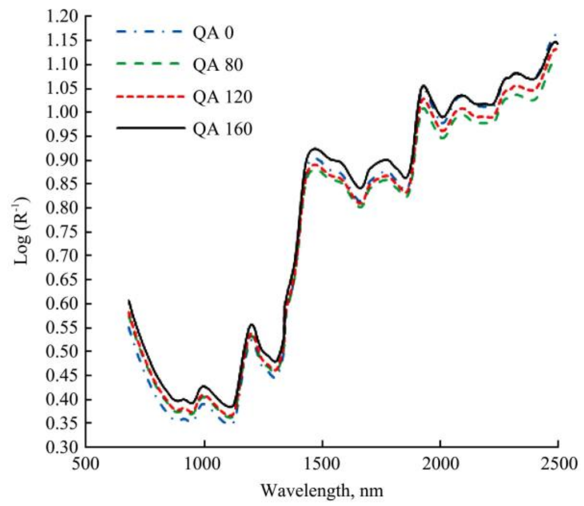
It is noticeable from the results of wheat quality characteristics in Table 1, especially protein ratio ranged from 10.23% to 13.44% for all varieties. In addition, the difference in the values of protein ratios, especially in the higher levels of nitrogen fertilization, is not large effectively. Where many researchers mentioned that wheat protein ratio from 10% to 14% classified as hard wheat and has specific food industries such as bread and pasta, unlike wheat protein ratio <10% is classified as soft wheat and used in other food industries such as cake (Cauvain and Cyster, 1996; Cauvain and Young, 2006; Delcour et al., 2012). Hence, if the optimum productivity and quality level of wheat grain have already been achieved, so there is no need for excessive nitrogen fertilization because it leading to more greenhouse gas especially nitrous oxide gas (N_2O), which is one of the most dangerous greenhouse gases that affect badly the environment. So, plant varieties breeders should be encouraged to develop wheat varieties capable of achieving productivity and quality optimum with the lowest level of nitrogen fertilization.

3.2 NIR spectroscopy method

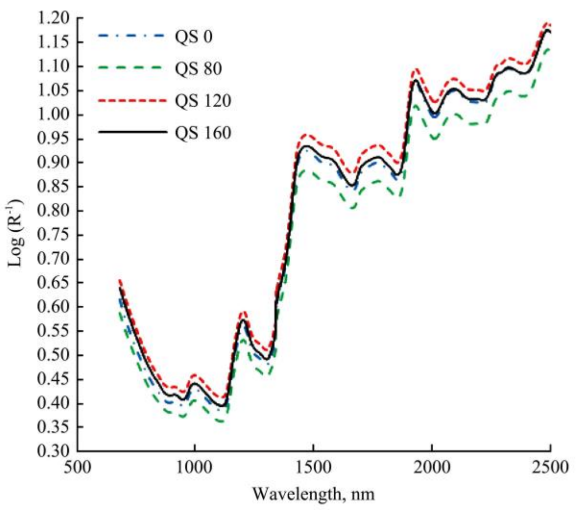
Figure 1a shows the scanned diversity of all wheat varieties in this study and exhibits the all raw spectra in a relationship between wavelength (nm) and the absorbance log (R^{-1}). While, Figure 1(b, c, and d) shows the mean spectrum for the whole wheat grain varieties of Alföld (QA), Mv Suba (QS), and Mv Toborzó (QT) under N fertilization 0, 80, 120 and 160 kg ha^{-1} respectively. Along the NIR region used, the all wheat grain varieties at fertilization levels 0, 80, 120 and 160 kg ha^{-1} showed different absorbance values, as it shown Figure 1(b, c, and d), this is due to the different rates of nitrogen fertilization added, which resulted in differences in the concentration of protein, gluten, moisture content and starch of wheat varieties under study.



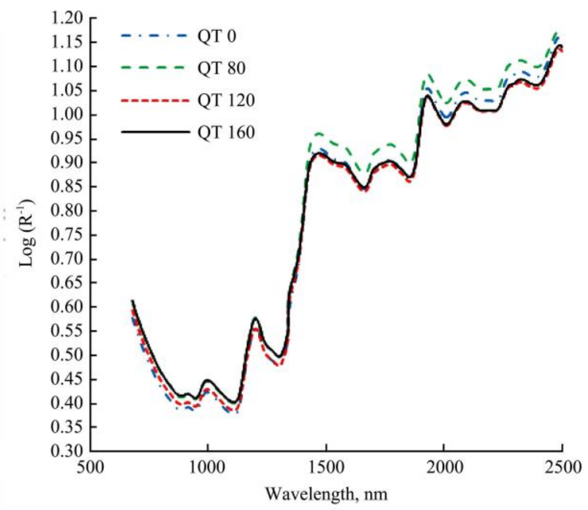
a. Raw spectra for all wheat varieties samples



b. The mean spectrum for Alföld (QA)



c. The mean spectrum for Mv Suba (QS)



d. The mean spectrum for Mv Toborzó (QT)

Figure 1 NIR spectral data

In the NIR region, all wheat quality parameters were characterized by peaks in the regions around 870, 980, 1180, 1450, 1750, 1920, 2070, 2300 and 2470 nm. The major absorption bands in the NIR region are attributable to the contribution of protein (1450, 1750, 2070, and 2300 nm), water (870, 980, 1180, 1450, and 1920 nm) and starch (980, 1450, 1750, 2300, and 2470 nm). These mentioned bands for the protein and gluten, water, and starch were respectively identified as 1st and 2nd overtones of N-H and C-H stretch, 1st, 2nd and 3rd overtone of O-H and C-H stretch, and 2nd and 3rd overtone of O-H stretch, C-H stretch/CH_2 deformation combination according to (Gergely and Salgó, 2005; Hacisalihoglu et al., 2010; Lin et al., 2014). Quality characteristics of different wheat varieties treated by nitrogen fertilization levels (0, 80, 120 and 160 kg ha^{-1}) were monitored using NIR waves ranged

680 to 2500 nm in order to development a calibration model to non-destructive quantification the content of both protein, gluten, moisture and starch, presented in Table 3.

Table 3 Effect of wavelengths range and pretreatment methods on the performance of PLS calibration models for predicting protein, gluten, moisture content and starch of wheat grain varieties

Pretreatment Methods		Protein, %			Gluten, %			Moisture content, %			Starch, %		
		NIR. Intervals, nm			NIR. Intervals, nm			NIR. Intervals, nm			NIR. Intervals, nm		
		Reg.(1)	Reg.(2)	Reg.(3)	Reg.(1)	Reg.(2)	Reg.(3)	Reg.(1)	Reg.(2)	Reg.(3)	Reg.(1)	Reg.(2)	Reg.(3)
Without treatments	SEC	0.61	0.55	0.59	1.2	1.8	1.58	0.21	0.23	0.23	0.62	0.57	0.56
	R_C^2	0.54	57	0.54	0.83	0.61	0.71	0.7	0.63	0.64	0.59	0.63	0.63
	SECV	0.74	0.64	0.67	1.75	1.98	1.74	0.23	0.25	0.25	0.71	0.62	0.62
	R_{CV}^2	0.43	0.51	0.49	0.64	0.55	0.65	0.63	0.56	0.57	0.43	0.56	0.56
	PCs	6	6	6	6	6	6	6	6	6	6	6	6
S. Golay	SEC	0.12	0.11	0.13	0.31	0.24	0.24	0.04	0.03	0.03	0.18	0.15	0.16
	R_C^2	0.98	0.98	0.98	0.99	0.99	0.98	0.99	0.99	0.99	0.96	0.97	0.97
	SECV	0.18	0.17	0.19	0.47	0.39	0.39	0.05	0.05	0.05	0.28	0.22	0.23
	R_{CV}^2	0.96	0.96	0.95	0.97	0.98	0.97	0.98	0.98	0.98	0.92	0.94	0.93
	PCs	6	6	6	6	6	6	6	6	6	6	6	6
MSC	SEC	0.33	0.42	0.44	0.88	1.5	1.5	0.13	0.19	0.16	0.35	0.42	0.47
	R_C^2	0.85	0.76	0.73	0.91	0.73	0.75	0.88	0.74	0.81	0.86	0.79	0.74
	SECV	0.43	0.47	0.5	1.19	1.69	1.7	.16	0.22	0.19	0.47	0.5	0.53
	R_{CV}^2	0.74	0.7	0.66	0.84	0.67	0.68	0.82	0.67	0.76	0.75	0.71	0.68
	PCs	6	6	6	6	6	6	6	6	6	6	6	6
SNV	SEC	0.34	0.42	0.44	0.90	1.5	1.5	0.13	0.19	0.16	0.36	0.42	0.47
	R_C^2	0.84	0.76	0.73	0.90	0.73	0.75	0.88	0.74	0.81	0.85	0.79	0.75
	SECV	0.44	0.47	0.5	1.21	1.7	1.7	0.16	0.22	0.19	0.48	0.5	0.53
	R_{CV}^2	0.74	0.7	0.66	0.83	0.67	0.68	0.82	0.67	0.76	0.74	0.71	0.68
	PCs	6	6	6	6	6	6	6	6	6	6	6	6

Note: S. Golay: Savitzky-Golay first derivative, R_{CV}^2: coefficient of determination for cross validation, PCs: principal components.

From the raw spectral (without pretreatment) and the three mathematical pretreatments (SG, MSC and SNV), it clearly showed that the SG pretreatment gave the best calibration model for all wheat quality characteristics at the three intervals NIR wavelength used, while the model without any pretreatments recorded the lowest results for all wheat quality characteristics. Where, the best result for protein and gluten was noted at wavelength Reg.(2) (1000 to 2500 nm), SECV and R_{CV}^2 were 0.17, 0.96 and 0.39, 0.98 respectively. While the moisture content, recorded the best value at all wavelength interval (680 to 2500 nm) by values, 0.05 and 0.98 for SECV and R_{CV}^2. Finally, the best values of SECV and R_{CV}^2 0.22 and 0.94 for starch content was observed at wavelength interval Reg. 2 (1000 to 2500 nm).

It can be seen from the above analysis that, the higher correlations between NIRS within range 680 to 2500 nm and chemical composition of wheat grain varieties treated by different nitrogen fertilization. Evidently, from the statics of calibration model in Table 3 that the best NIR wave interval and mathematical pretreatment method for protein, gluten, moisture content and starch of all wheat varieties studied thus, the best model could be predicted by the highest value of R_{CV}^2 and the lowest SECV for each of wheat quality characteristics under study. To be sure the calibration model advantages of outlined in the previous paragraph, an external validation process was applied to verify the precision of calibration model performance, in order to prediction and quantification protein, gluten, moisture content and starch for wheat grain varieties, and the statistics obtained from verifying operation were tabulated in Table 4 and illustrated in Figure 2.

Table 4 External validation statistics for protein, gluten, moisture content and starch using the global calibration equations

Wheat quality characteristics	NIR Interval, nm	Pretreatment method	Range	Mean	SD	Model precision indicators			
						R_P^2	SEP	RPD	Bias
Protein, %	1000 : 2500	S.Golay	10.23-13.38	12.1	1.05	0.96	0.17	6.25	-0.12^{-2}
Gluten, %	1000 : 2500	S.Golay	24.25-32.46	29.48	2.56	0.98	0.39	6.53	-0.94^{-2}
Moisture content, %	680 : 2500	S.Golay	9.33-10.53	9.9	0.47	0.98	0.05	9.79	-0.9^{-3}
Starch, %	1000 : 2500	S.Golay	63.19-66.10	64.44	1.06	0.94	0.22	4.82	-0.11^{-2}

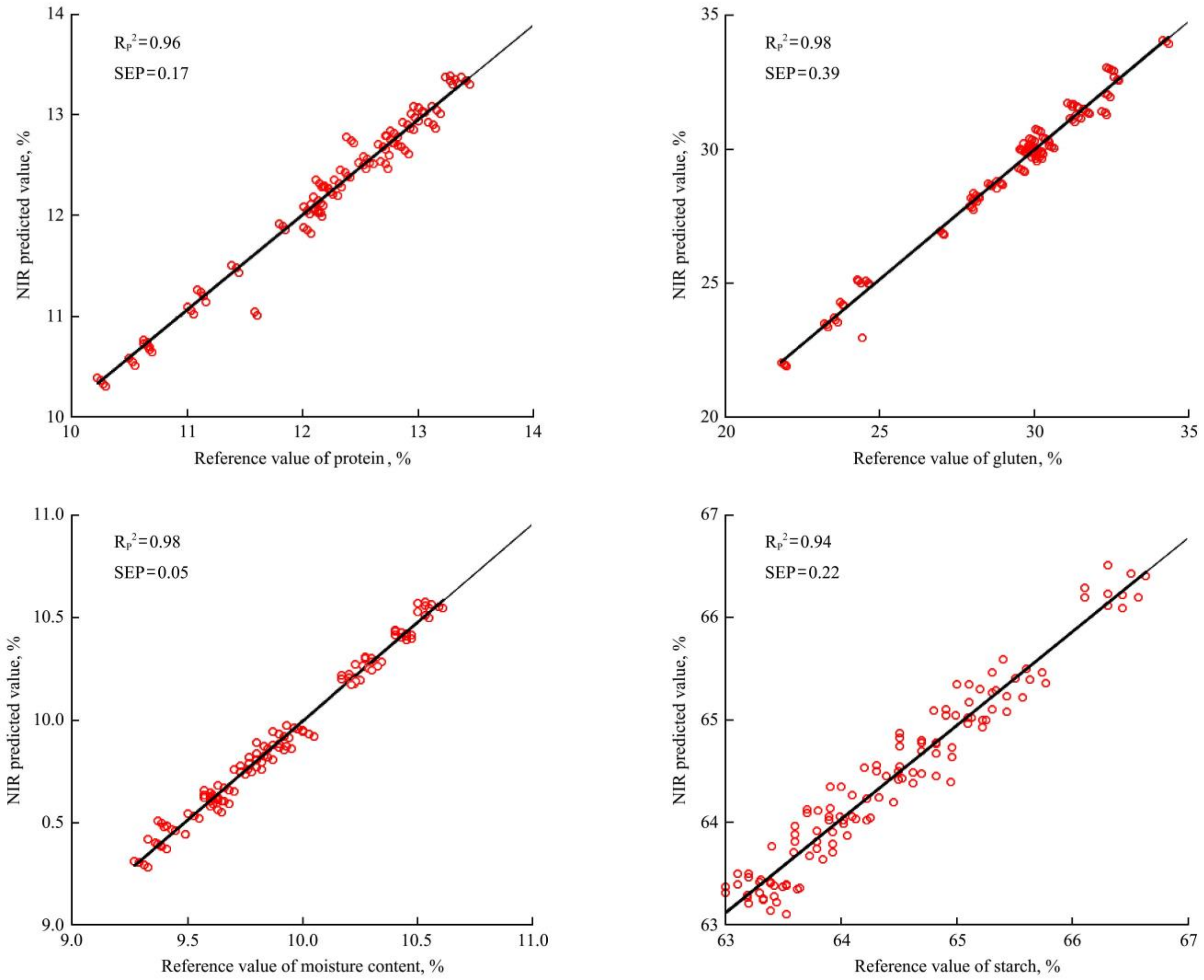


Figure 2 Illustrated the precision of the NIR model for calibration and quantification protein, gluten, moisture content and the starch reference values vs. NIR predicted values

As observed from Table 4 that the quality characteristics of protein, gluten, moisture content and the starch for all wheat grain varieties under the study with mathematical pretreatment S.Golay in all analyses resulted in a model with the best precision. Based on mentioned in the preceding paragraph, it was found that the calibration established for monitoring some quality attributes of different wheat varieties from the NIR-wave region ranged from 1000 to 2500 and from 680 to 2500 nm (as mentioned in Table 3) for protein, gluten, starch and moisture content respectively, showed higher precision, indicated by higher R_P^2 and RPD and lower SEP. Where, the lower value of SEP observed at moisture content while the high value was at gluten and also the higher value of R_P^2 noted at moisture content and gluten by the same value and followed by the values of each protein and starch respectively as showed in Table 4. Likewise, RPD recorded the best values for moisture content, gluten, protein, and starch according to Table 4, where, RPD values ranged from 4.82 to 9.79 for the various parameters indicating that the NIR measurements should be useful in quality control applications.

4 Conclusions

Infrared technology as a non-destructive method for monitoring and assessing quality attributes of wheat grains has the potential to replace the traditional methods to estimate the protein, gluten, moisture content, starch and other quality characteristics that affect the occupational health and safety for technicians and researchers in addition to time, effort consuming and generate chemical waste. The NIR model were developed to monitor wheat quality characteristics was achieved the best prediction performance through the values of R_P^2, SEP, RPD and bias, 0.96, 0.17, 6.25 and -1.2×10^{-3} for protein and also gluten the values were 0.98, 0.39, 6.53 and -9.4×10^{-3} while the moisture content recorded 0.98, 0.05, 9.79 and -9×10^{-4}, in the final the values of starch were 0.94, 0.22, 4.82 and -1.1×10^{-3}. Considering the overall results indicators, it could be said that NIR techniques can be effectively applied to monitor the quality of wheat and quantification a lot of wheat quality attributes.

References

AACC. 2000. *Approved Methods of the American Association of Cereal Chemists, 10th ed.* St. Paul, American Association of Cereal Chemists Inc.

Alam, M. S., M. N. Nesa, S. K. Khan, M. B. Hossain, and A. Hoque. 2007. Varietal differences on yield and yield contributing characters of wheat under different levels of nitrogen and planting methods. *Journal of Applied Sciences Research,* 3(11): 1388–1392.

Beman, J. M., K. R. Arrigo, and P. A. Matson. 2005. Agricultural runoff fuels large phytoplankton blooms in vulnerable areas of the ocean. *Nature*, 434(7030): 211–214.

Blandino, M., F. Marinaccio, P. Vaccino, and A. Reyneri. 2015. Nitrogen fertilization strategies suitable to achieve the quality requirements of wheat for biscuit production. *Agronomy Journal*, 107(4): 1584–1594.

Burns, D. A., and E. W. Ciurczak. 2001. *Handbook of Near-Infrared Analysis*. New York: Marcel Dekker.

Cassells, J. A., R. Reuss, B. G. Osborne, and I. J. Wesley. 2007. Near infrared spectroscopic studies of changes in stored grain. *Journal of Near Infrared Spectroscopy*, 15(3): 161–167.

Cauvain, S. P., and J. A. Cyster. 1996. *Sponge Cake Technology*. Chipping Campden: CCFRA.

Cauvain, S. P., and L. S. Young. 2006. *Baked Products: Science, Technology and Practice*. Oxford: Wiley-Blackwell.

Delcour, J. A., I. J. Joye, B. Pareyt, E. Wilderjans, K. Brijs, and B. Lagrain. 2012. Wheat gluten functionality as a quality determinant in cereal-based food products. *Annual Review of Food Science and Technology,* 3(1): 1–24.

Dowell, F. E., E. B. Maghirang, F. Xie, G. L. Lookhart, R. O. Pierce, B. W. Seabourn, S. R. Bean, J. D. Wilson, and O. K. Chung. 2006. Predicting wheat quality characteristics and functionality using near-infrared spectroscopy. *Cereal Chemistry,* 83(5): 529–536.

Dupont, F. M., and S. B. Altenbach. 2003. Molecular and biochemical impacts of environmental factors on wheat grain development and protein synthesis. *Journal of Cereal Science*, 38(2): 133–146.

Ferreira, D. S., O. F. Galão, J. A. L. Pallone, and R. J. Poppi. 2014. Comparison and application of near-infrared (NIR) and mid-infrared (MIR) spectroscopy for determination of quality parameters in soybean samples. *Food Control*, 35(1): 227–232.

Food and Agriculture Organization (FAO). 2009. *Global Agriculture towards 2050*. Rome, Italy: FAO.

Gauer, L. E., C. A. Grant, D. T. Gehl, and I. D. Balley. 1992. Effects of nitrogen fertilization on grain protein content, nitrogen uptake and nitrogen use efficiency of six spring wheat (Triticum aestivum L.) cultivars in relation to estimated moisture supply. *Canadian Journal of Plant Science*, 72(1): 235–241.

Gergely, S., and A. Salgó. 2003. Changes in moisture content during wheat maturation-what is measured by near infrared spectroscopy? *Journal of Near Infrared Spectroscopy*, 11(1): 17–26.

Giller, K. E., P. M. Chalk, A. Dobermann, L. C. Hammond, P. Heffer, J. K. Ladha, P. Nyamudeza, L. M. Maene, H. Ssali, and J. R. Freney. 2004. Emerging technologies to increase the efficiency of use of fertilizer nitrogen. In *Agriculture and the Nitrogen Cycle: Assessing the Impacts of Fertilizer Use on Food Production and the Environment*, A. R. Mosier, et al., eds. 35–52. Washington, D. C.: Island Press.

Hacisalihoglu, G., B. Larai, and A. M. Settles. 2010. Near-infrared reflectance spectroscopy predicts protein, starch, and seed weight in intact seeds of common bean (Phaseolus vulgaris L.). *Journal of Agricultural and Food Chemistry*, 58(2): 702–706.

Igne, B., and C. R. Hurburgh. 2010. Local chemometrics for samples and variables: optimizing calibration and standardization processes. *Journal of Chemometrics*, 24(1-2): 75-86.

Johansson, E., M. L. Prieto-Linde, and G. Svensson. 2004. Influence of nitrogen application rate and timing on grain protein composition and gluten strength in Swedish wheat cultivars. *Journal of Plant Nutrition and Soil Science*, 167(3): 345–350.

Lin, C., X. Chen, L. Jian, C. Shi, X. Jin, and G. Zhang. 2014.

Determination of grain protein content by near-infrared spectrometry and multivariate calibration in barley. *Food Chemistry*, 162(6): 10–15.

Long, D. S., R. E. Engel, and M. C. Siemens. 2008. Measuring grain protein concentration with in-line nir reflectance spectroscopy. *Agronomy Journal*, 100(2): 247–252.

Maertens, K., P. Reyns, and J. D. Baerdemaeker. 2004. On-line measurement of grain quality with NIR technology. *American Society of Agricultural Engineers*, 47(4): 1135–1140.

Miralbes, C. 2008. Discrimination of European wheat varieties using near infrared reflectance spectroscopy. *Food Chemistry*, 106(1): 386–389.

Montes, J. M., H. F. Utz, W. Schipprack, B. Kusterer, J. Muminovic, and C. Paul. 2006. Near-infrared spectroscopy on combine harvesters to measure maize grain dry matter content and quality parameters. *Plant Breeding*, 125(6): 591–595.

Osborne, B. G. 2000. Recent developments in NIR analysis of grains and grain products. *Cereal Foods World*, 45(1): 11–15.

Ottman, M. J., T. A. Doerge, and E. C. Martin. 2000. Durum grain quality as affected by nitrogen fertilization near anthesis and irrigation during grain filling. *Agronomy Journal*, 92(5): 1035–1041.

Petiscoa, C., B. García-Criadoa, B. R. Vázquez-de-Aldanaa, A. de Harob, and A. García-Ciudada. 2010. Measurement of quality parameters in intact seeds of Brassica species using visible and near-infrared spectroscopy. *Industrial Crops and Products*, 32(2): 139–146.

Rinnan, A., F. V. D. Berg, and S. B. Engelsen. 2009. Review of the most common preprocessing techniques for near-infrared spectra. *Trends in Analytical Chemistry*, 28(10): 1201–1222.

Zhao, C., M. He, Z. Wang, Y. Wang, and Q. Lin. 2009. Effects of different water availability at post-anthesis stage on grain nutrition and quality in strong-gluten winter wheat. *Comptes Rendus Biologies*, 332(8): 759–764.