[International Journal of Business and Technology](https://knowledgecenter.ubt-uni.net/ijbte)

Volume 9
Issue 1 *Spring 2021*

Article 18

March 2021

Soft wheat quality parameters evaluation by Near Infrared Spectroscopy: from field to shelf analysis

Kliton Bylykbashi
University for Business and Technology - UBT, kliton.bylykbashi@ubt-uni.net

Recommended Citation

Bylykbashi, Kliton (2021) "Soft wheat quality parameters evaluation by Near Infrared Spectroscopy: from field to shelf analysis," *International Journal of Business and Technology*: Vol. 9: Iss. 1, Article 18.
DOI: 10.33107/ijbte.2021.6.3.16
Available at: https://knowledgecenter.ubt-uni.net/ijbte/vol9/iss1/18

Soft wheat quality parameters evaluation by Near Infrared Spectroscopy: from field to shelf analysis

Giuseppe Bonifazi[1,2], Riccardo Gasbarrone[1], Silvia Serranti[1,2], Kliton Bylykbashi[3]

[1] Department of Chemical Engineering Materials Environment,
Sapienza University of Rome, Italy
{giuseppe.bonifazi, silvia.serranti}@uniroma1.it

[2] Research Center for Biophotonics, Sapienza University of Rome,
Polo Pontino, Italy
{giuseppe.bonifazi, riccardo.gasbarrone
silvia.serranti}@uniroma1.it

[3] UBT, Prishtina, Kosove
kliton.bylykbashi@ubt-uni.net

Abstract. Near InfraRed Spectroscopy (NIRS) is a powerful tool that is widely applied in agro-food science and technology research for qualitative as well as quantitative analysis. It is one analytical technique that is taking place in this sector due to its low costs, reliability, rapidity and not invasive / non-destructive nature. NIRS along with chemometric modelling can provide accurate assessment of various grain quality attributes and the chemical composition of grain. The present work investigates the ability of using NIRS for the evaluation of different wheat quality parameters by using a portable spectroradiometer working in Visible – Short Wave InfraRed (Vis-SWIR: 350 – 2500 nm) spectral range. The potential of NIR-based techniques for predicting moisture content (12.6 ± 0.4 %), specific gravity (79.4 ± 2.7 kg/hl), protein content (14.0 ± 1.8 %), wet gluten content (28.1± 4.2 %), W index or Flour strength (266.3 ± 92.2) and hardness (60.3 ± 20.8 %) is explored. Present findings show the reliability of using NIRS as a quality control tool not only at laboratory scale, from the mill plant point of view (i.e. by acquiring reflectance spectra on wheat flour arranged in Petri dish), but even in on-line industrial application and shelf storage control evaluation, from the bakery plant / consumers' point of view (i.e. by acquiring reflectance spectra on wheat flour sack).

Keywords: Near Infrared Analysis, Partial Least Squares regression, soft wheat flour, Principal Component Analysis, quality control.

1 Introduction

The quality of produced soft wheat flour might vary, because it is obtained by grinding together different kind of wheat and sometimes using same mixture in different ratios [1]. Indeed, each producer needs to be supplied with a standard quality of wheat as raw material for its production. The entire production could be lost generating a great economic loss if the characteristics of the supplied wheat doesn't respect the requirement standards characteristics. It is thus of mandatory importance, on the side of farmer to perform quality control on stored batch, and, on the side of the milling plant / processor, to continuously control supplied batch and assessing the quality of the product processing.

At present chemical-analytical methods, that are mainly destructive and invasive methods, are widely used to perform grain quality estimation at grain handling facilities. However, these methods are not efficient and are cost- and/or time- consuming. For this reason, there is a need of an automated, cost-saving, rapid, not-destructive and not-invasive method for estimating grain quality [2]. Near InfraRed (NIR) spectroscopy technique have been successfully applied for evaluating different quality parameters of agro-food industry products [3-5]. The utilization of NIRS for performing quality evaluation on wheat grain have been investigated by different authors for predicting protein content, starch content and other quality parameters [6-9]. Is it evident how the role of NIRS in cereal processing and, more in general in food quality applications, is becoming more and more central. NIRS represents a simple, rapid and accurate method for nondestructive measurement of multiple attributes of the wheat. Due to that, it is not surprising that the NIRS-based method, coupled with chemometrics technique has been accepted as a standard method by ISO and others (i.e. AACC, AOAC and ICC) [10].

In this scenario, NIRS, together with multivariate statistics, could be seen as an alternative method to conventional ones for evaluating quality control parameters of wheat flour. So, the main goal of this research is to apply a non-destructive method like NIR coupled with chemometric techniques as an alternative procedure to destructive methods in order to assess different quality parameters of different kind of soft wheat grains. The ability of a spectroradiometer, working in Visible – Short Wave InfraRed (Vis-SWIR: 350-2500 nm), for predicting moisture content, specific gravity, protein content, wet gluten content, W index or Flour strength and hardness was tested. Multivariate regression models were calibrated using reference parameters and reflectance spectra collected on wheat arranged in Petri dishes.

2. Materials and methods

2.1 Analyzed materials and samples presentation

In this study, four different kind of wheat samples were analyzed (Figure 1): a) French soft wheat, b) Romanian soft wheat, c) Northern Spring soft wheat and d) Ukrainian proteic soft wheat. As shown in Table 1, for each given soft wheat

https://knowledgecenter.ubt-uni.net/ijbte/vol9/iss1/18
DOI: 10.33107/ijbte.2021.6.3.16

sample were measured and calculated the following parameters as references: moisture content (12.6 ± 0.4 %), specific gravity (79.4 ± 2.7 kg/hl), protein content (14.0 ± 1.8 %), wet gluten content (28.1± 4.2 %), W index (266.3 ± 92.2) and hardness (60.3 ± 20.8 %).

a b c d

Fig. 1. Analyzed soft wheat flour samples: a) French soft wheat ("*B – Grano tenero Francese*"), b) Romanian soft wheat ("*C – Grano tenero Romeno*"), c) Northern Spring soft wheat ("*H –Grano tenero Northern Spring*"), and d) Ukrainian proteic soft wheat ("*G – Grano tenero Ucraino proteico*").

Table 1. Reference measurements for the soft wheat samples.

Sample ID	*Grano tenero Francese*	*Grano tenero Romeno*	*Grano tenero Northern Spring*	*Grano tenero Ucraino proteico*
Product	French soft wheat	Romanian soft wheat	Northern Spring soft wheat	Ucranian proteic soft wheat
Moisture content (%)	12.4	12.1	13.1	12.7
Specific gravity (kg/hl)	77.9	78.8	83.4	77.4
Protein content (%)	12.4	12.4	15	16
Wet gluten content (%)	24.6	24.5	30.6	32.8
W Index	226	157	321	361
Hardness (%)	65	32	62	82

2.2 Portable spectroradiometer system, calibration procedure and reflectance spectra acquisition

Twenty spectra acquisitions in reflectance mode were performed using the ASD FieldSpec 4 ® Standard-Res field portable spectroradiometer [11] for each of the 4 sample in Petri dish (number of spectra = 80). Sample presentation mode to the spectrometer was in reflectance. The measurements were performed by putting the contact probe on the top surface of Petri plates in which wheat kernels were arranged. The used portable instrument, that consists of a detectors case and a 1.5 m fiber optic cable coupled with a contact probe, is able of recording spectra based on the information of 2151 bands in Vis-SWIR regions (350 – 2500 nm), with a spectral resolution of 3 nm at 700 nm and 10 nm at 1400/2100 nm. Data records and the calibration procedure were performed using the ASD RS^3 software.

2.3 Data handling and chemometric modelling

Spectral data handling, pre-processing and exploratory analysis. Collected data were imported into MATLAB® environment (MATLAB R2018a; The Mathworks) by using an ad hoc written script and thus analyzed using the PLS_toolbox (ver. 8.2.1; Eigenvector Research, Inc) in MATLAB® environment. Data were stored into datasets objects (DSO) and classes were set. Reflectance data were pre-processed for removing the noisiest parts of the spectra and to enhance differences occurring among clusters of data classes [12]. The pre-process combination used was Splice Correction (SC), Norris-Williams (NW) Gap Segment 2nd Derivative, Standard Normal Variate (SNV) and Mean Center (MC). The SC pre-process algorithm was used for eliminating the gaps in the acquired signals, located at λ =1000 nm and λ = 1800nm, between the domains of the different detector arrays [13]. NW derivation was performed to avoid the noise inflation in finite differences. While SNV was used to correct scatter artifacts [12, 14]. Finally, MC was used to centers columns to have zero mean [14].

Principal Component Analysis, a chemometric technique that is able to extract the dominants patterns of the reflectance spectra data matrix X, was chosen to perform the exploratory analysis of decomposed spectra data, according to sample type and for excluding outliers from the datasets [15].

Partial Least Squares (PLS) Regression. Partial Least Squares (PLS) regressions were performed to evaluate the correlation between each of the considered parameters (shown in Table 1) Y, and the reflectance spectra X, collected on the wheat kernels arranged in Petri dish. The PLS regression is a chemometric technique that is generally used when a set of dependent variables, stored in the matrix Y of responses, have to be predicted from a large set of independent variables, that are stored in the matrix X of predictors [16]. Each dataset was thus randomly split into two parts by using Euclidean-based Kennard/Stone (K/S) algorithm [17]. The 70% of the data was used as training set, while the remaining data percentage (30%) was used as test set for the PLS regression. Firstly, the PLS models were calibrated and cross-validated by using Venetian Blinds as cross-validation method for assessing the optimal complexity of the model and choosing the number of Latent variables (LVs) [14]. Then test sets were used for validation. The main parameters used for evaluating the goodness of regression models [15] were: i) the Root Mean Square Error in Prediction (RMSEP), ii) the coefficient of determination R_p^2 and iii) the Bias.

3. Results and discussion

The raw reflectance spectra, that were used for building the PLS regressions, averaged according to the analyzed samples of soft wheat kernels in Petri dish are shown in Figure 2. As a result, the built regression models have shown a

https://knowledgecenter.ubt-uni.net/ijbte/vol9/iss1/18
DOI: 10.33107/ijbte.2021.6.3.16

significant ability to predict the reference parameters of the soft wheat kernels in petri dishes, as shown from the performance parameters shown in Table 2.

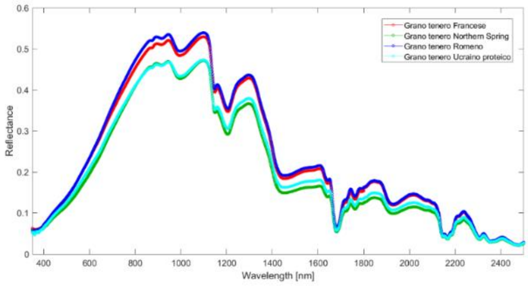

Fig. 2. Grand-average raw reflectance spectra of soft wheat kernels in Petri dish.

Table 2. Regression models parameters for the soft wheat samples in Petri dish. LV = Latent Variables; RMSEC = Root Mean Squared Error Calibration; RMSECV = Root Mean Squares Error Cross Validation; RMSEP = Root Mean Squared Error Prediction; R^2 (Cal) = coefficient of determination in calibration; R^2 (CV) = coefficient of determination in cross-validation; R^2 (Pred) = coefficient of determination in prediction.

	Hardness (%)	**Wet gluten (%)**	**Specific gravity (kg/hl)**	**Protein (%)**	**Moisture (%)**	**W**
LV	9	5	9	4	8	7
RMSEC	2.3	1.1	0.3	0.5	0.0	11.6
RMSECV	8.6	1.5	1.1	0.5	0.1	31.0
RMSEP	4.2	1.3	0.9	0.5	0.1	22.6
R^2 (Cal)	0.985	0.911	0.987	0.917	0.993	0.979
R^2 (CV)	0.789	0.845	0.754	0.897	0.954	0.853
R^2 (Pred)	0.935	0.874	0.908	0.922	0.885	0.905

4. Conclusions and future perspective

The ability of a spectroradiometer working in Visible – Short Wave InfraRed (350-2500 nm) for predicting moisture content, specific gravity, protein content, wet gluten content, W index or flour strength and hardness was explored. Multivariate regressions for predicting different wheat grain quality parameters were calibrated and validated, showing promising performance for predicting wheat grain quality attributes from reflectance spectra. However, further studies should be carried out for developing NIRS-based calibration and prediction models to assess quality parameters of wheat grains using many other wheat varieties. Following this approach, it could be possible to define innovative strategies to state different parameters of soft wheat grain in food quality control process. This should be addressed also in a decision-making perspective: on the side of farmer to perform quality control on stored – to be supplied batch, and, on

5

the side of the milling plant / processor, to continuously control supplied batch and assessing the quality of the product processing. Quality control over wheat grain can be applied, without the need of wet-chemistry laboratory analysis in a fastest and as well reliable way.

References

[1] Varzakas T. (2016), Quality and Safety Aspects of Cereals (Wheat) and Their Products, Critical Reviews in Food Science and Nutrition, 56:15, 2495-2510.
[2] Singh, C.B., Paliwal, J., Jayas, D.S. and White, N.D.G. (2006), "Near-infrared spectroscopy: Applications in the grain industry" Paper No. 06-189. CSBE/SCGAB 2006 Annual Conference, Edmonton Alberta. July 16 - 19, 2006.
[3] Bart, M. N., Beullens, K., Bobelyn, E., Peirs, A., Saeys, W., Theron, K. I. and Lammertyn, J. (2007), "Nondestructive measurement of fruit and vegetable quality by means of NIR spectroscopy: A review," Postharvest Biology and Technology, 46, 99–118.
[4] Serranti, S., Bonifazi, G., Gasbarrone, R. (2018), "Kiwifruits ripening assessment by portable hyperspectral devices", Proc. SPIE 10665, Sensing for Agriculture and Food Quality and Safety X, 106650S (15 May 2018).
[5] Serranti, S., Bonifazi, G., Gasbarrone, R. (2018), "Olive fruit ripening evaluation and quality assessment by hyperspectral sensing devices", Proc. SPIE 10665, Sensing for Agriculture and Food Quality and Safety X, 106650R (15 May 2018).
[6] Delwiche, S. R. and Hruschka, W. R. (2000), "Protein Content of Bulk Wheat from Near-Infrared Reflectance of Individual Kernels". Cereal Chemistry, 77: 86-88.
[7] Cozzolino, D., Scott, D. and Eglinton, J. K. (2014). "A Review on the Role of Vibrational Spectroscopy as An Analytical Method to Measure Starch Biochemical and Biophysical Properties in Cereals and Starchy Foods." Foods.
[8] Millar, S. J. (2003), "The Development Of Near Infrared (Nir) Spectroscopy Calibrations For The Prediction Of Wheat And Flour Quality", Home-Grown Cereals Authority (HGCA) Project Report No. 310. August 2003
[9] Pojić, M., Mastilović, J. and Majcen, N. (2012). "The Application of Near Infrared Spectroscopy in Wheat Quality Control", Infrared Spectroscopy - Life and Biomedical Sciences.
[10] ISO 12099:2017. "Animal feeding stuffs, cereals and milled cereal products — Guidelines for the application of near infrared spectrometry" (2017).
[11] ASD Inc. (2015), "FieldSpec® 4 User Manual, ASD Document 600979, Rev. D" (June 2015).
[12] Danner, M., Locherer, M., Hank, T. and Richter, K. (2015), "Spectral Sampling with the ASD FieldSpec 4 –Theory, Measurement, Problems, Interpretation". EnMAP Field Guide's Technical Report, GFZ Data Services.
[13] Rinnan, Å., van den Berg, F. and Engelsen, S.B. (2009), "Review of the most common pre-processing techniques for near-infrared spectra," Trends in Analytical Chemestry, 28, 10.
[14] Wise, B. M., Gallagher, N. B., Bro, R., Shaver, J. M., Windig, W., Koch, R.S. (2008), "PLS_Toolbox 4.2 Reference Manual for use with MATLAB™," West Eaglerock Drive, Wenatchee, WA: Eigenvector Research Incorporated Inc.
[15] Wold, S., Esbensen, K. and Geladi, P. (1987), "Principal Component Analysis," Chemometrics and Intelligent Laboratory Systems, 2, 37-52.
[16] Abdi, H., "Partial Least Squares (PLS) Regression," In: Lewis-Beck M., Bryman, A., Futing T. (Eds.). Encyclopedia of Social Sciences Research Methods. Thousand Oaks (CA): Sage. (2003).
[17] Kennard, R.W. and Stone, L.A. (1969), "Computer-aided Design of Experiments". Technometrics, 11, 137-148.

https://knowledgecenter.ubt-uni.net/ijbte/vol9/iss1/18
DOI: 10.33107/ijbte.2021.6.3.16