ON-COMBINE NEAR INFRARED SPECTROSCOPY APPLIED TO PREDICTION OF GRAIN TEST WEIGHT

D.J. Bonfil[1], I. Mufradi[1], S. Asido[1] and D.S. Long[2]

1. *Field Crops and Natural Resources Department*
Agricultural Research Organization
Gilat Research Center, MP Negev 85280, Israel

2. *Columbia Plateau Conservation Research Center*
USDA-Agricultural Research Service
Pendleton, OR 97810, USA

ABSTRACT

Whole grain near infrared (NIR) spectroscopy is a widely accepted method for analysis of the protein and moisture contents of grain, but is seldom applied to predict test weight. Test weight is a widely used specification for grading of wheat and predictor of flour yield. The objective of this study was to determine whether NIR spectroscopy could be used for measuring the test weight of grain. Reference grain samples of hard red spring wheat were obtained from dryland fields in the semiarid Negev region of Israel. Two NIR optical instruments were used: the laboratory Foss NIRS 6500 spectrometer that measures spectral reflectance from 400 to 2498 nm and the on-combine Zeltex AccuHarvest Grain Analyzer that measures spectral transmittance from 893 to 1045 nm (14 channels). Near infrared spectroscopy showed potential for predicting test weight (R^2 < 0.88) with accuracies suitable for mapping the spatial variability of this grain quality attribute in the field. This post-harvest information will be potentially useful for yield map interpretation.

Keywords: Crop monitoring, Foss NIRS 6500, Zeltex AccuHarvest, Near infrared, On-the-go, Wheat.

INTRODUCTION

Whole grain near infrared (NIR) spectroscopy (Williams and Norris, 1987) is a widely accepted method for laboratory analysis of the protein and moisture contents of grain (Delwiche, 2004). Recently, this technology was adapted for use on a combine harvester for continuously measuring the protein concentration of wheat (*Triticum aestivum* L.) as the grain is conveyed through the threshing system and into the bulk tank (Long et al., 2005, Long and Rosenthal, 2005; Long et al., 2008).

Dowell et al. (Dowell et al., 2006) showed that bench-type NIR spectrometers, due to correlation with grain protein concentration, can be used to predict many grain quality traits, while test weight, a widely used specification for grading wheat and predicting flour yield, was one trait that could be predicted even when the influence of protein content was removed. Test weight measurements, when integrated with GPS technology, would enable test weight mapping of farm fields. This information may assist in the interpretation of accompanying grain yield maps. Plus, optical sensors might be used during harvest to segregate grain by test weight limits, thus enabling growers to better accommodate variability in grain quality traits and achieve consistently higher quality.

The official method of determining test weight of grain involves measuring the weight of wheat per standard (0.5 L) volume. Measurements may be obtained within 1-min with an accuracy of ±0.18 kg hL^{-1} (0.15 lb bu^{-1}). However, this laboratory-based approach would not be feasible for analyzing a large volume of samples as needed for spatial characterization. In the present study, on-combine NIR sensing was evaluated for ability to accurately measure and rapidly map test weight of grain within farm fields.

MATERIALS AND METHODS

Grain Samples

Reference grain samples of hard red spring wheat (n=1342) were obtained during machine harvest of dryland fields in the semiarid Negev region of Israel. Test weight determinations were accomplished in the laboratory by weighing a unit volume (0.25 L) of grain. These samples resulted in a wide range of test weight: 67-84 kg hL^{-1} (52-65 lbs bu^{-1}).

NIR Instrumentation

Two NIR optical instruments were evaluated in this study for the analysis of grain test weight. The first was a laboratory NIR spectrophotometer (Foss NIRS Model 6500, Silver Springs, MA, USA) and the second was designed for operation on a combine harvester (Zeltex AccuHarvest Grain Analyzer, Hagerstown, MA, USA). The NIRS 6500 is a precision instrument not designed for field use; however, it was included in this study for corroboration with Dowell et al. (2006) who found that it could predict test weight with R^2 = 0.74. It uses a mobile diffraction grating and is capable of scanning widely across the visible and NIR spectral regions (400-2498 nm). The NIRS 6500 measures NIR absorbance using diffuse reflectance. The AccuHarvest is a diode array instrument with 14 detectors that are capable of rapid scanning within the 893-1045 nm spectral region. Near infrared absorbance is measured using diffuse transmittance. Calibration is accomplished using the following regression specification:

$$\text{Test Weight} = \beta0 + \beta1(A1) + \beta2(A2) + \ldots \beta14(A14) + \beta15(Ta) + \beta16(Ts)$$

where $\beta 0$ is a bias term, $\beta 0$ through $\beta 16$ are slope coefficients, and A1 through A14 are spectral absorbances measured at each of the 14 wavelengths, and Ta and Ts are the ambient and sample temperatures at the time of measurement.

Spectroscopy and Data Analysis

The reference grain samples were divided into a calibration set and a validation set. For the NIRS 6500 instrument, spectral reflectance data were obtained by scanning a 20 g subsample 32 times with each scan recorded as log (1/R) in 2 nm intervals. All 32 scans were then averaged into one spectrum. Spectral analysis was undertaken using the Foss WinISI® II spectral analytical software. Prediction models were developed by a modified partial least squares (MPLS) regression on the first or second derivative of the absorbance log (1/R). During calibration, outliers were rejected using the software threshold default value. A one-sample-out cross validation procedure was used for the MPLS regression.

The AccuHarvest instrument calibration and validation were based on a subset (n=94) of the 1342 samples used for the NIRS 6500 calibration. Spectral data were obtained as the average of three scans of a 50 g grain sample that had been passed through the instrument. Prediction models were estimated by ordinary least squares (OLS) regression on the transmittance log (1/T). Multiple regression analyses were performed within the MS-Excel statistical software package. The resulting model parameters were then imported into the AccuHarvest Calibration software. The AccuHarvest was validated with data obtained when operated on a combine harvester during harvest. Maps of test weight derived from the sensor were visually compared with maps derived from 53 to 107 reference values. The reference values had been obtained from grain samples that had been sampled by hand at the grain bin filling auger of a combine during harvest.

The multiple coefficient of determination (R^2) and standard error of prediction (SEP), or standard deviation of the differences between NIR and reference values, were used to evaluate the accuracy of each instrument.

RESULTS AND DISCUSSION

Use of NIR Analysis for Test Weight

Best results for the NIRS 6500 instrument were obtained using a prediction model based on the second derivative of the spectral reflectance in the 400-2498 nm spectral region. Regression analysis yielded good results ($R^2 = 0.84$) with a standard error of prediction (SEP) of 0.99 kg hL^{-1} for test weight of hard red spring wheat (Fig. 1).

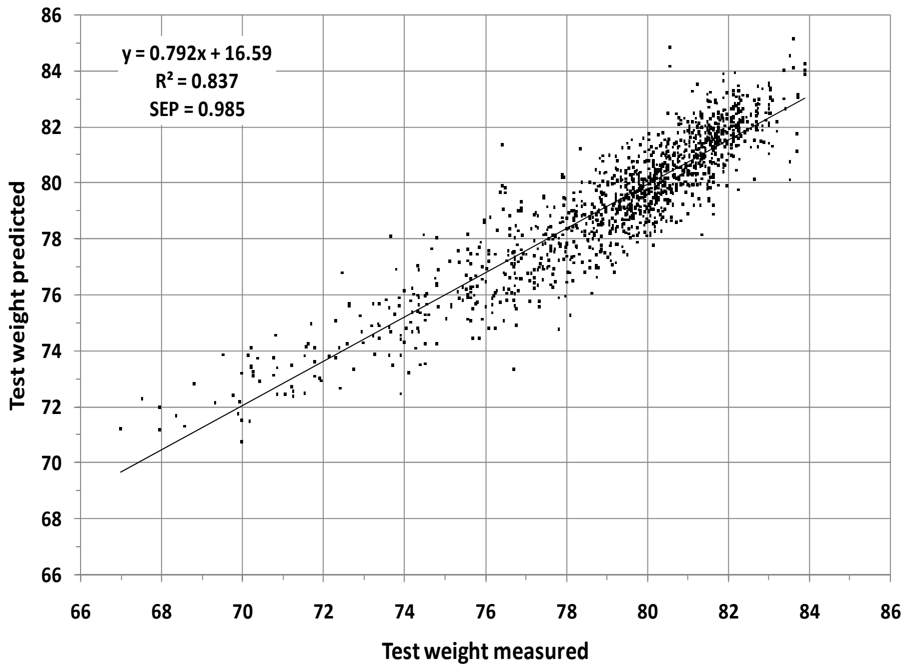

Figure 1. Correlations between measured test weight by common procedure (weighting 250 ml of grains) and predicted test weight by Foss-NIRS (reflectance of 20 g grains). n=1342.

The subset of grain samples (n=94) that was used for calibration of the AccuHarvest sensor spanned a wide range in test weight values (67 to 84 kg hL^{-1}). A calibration model was developed using the NIR spectral and test weight data from these 94 calibration samples. The predicted versus the reference test weight measurements were highly correlated (R^2 = 0.88) for the AccuHarvest bench calibration (Fig. 2). Measurement accuracy of NIR prediction by the AccuHarvest was similar to the NIRS 6500 (SEP = 1.3 kg hL^{-1} vs. 1.0 kg hL^{-1}).

An R^2 value between 0.7 and 0.9 would indicate an instrument that is suitable for rough screening, but not for quality control or process control (Williams, 2001). In addition, test weight measurements must be within a tolerance of ±0.15 lb bu^{-1} (0.18 kg hL^{-1}) in accordance with U.S. Federal Grain Inspection Service standards. Our results for the SEP greatly exceed this limit further indicating that NIR spectroscopy would not provide acceptable accuracy for process control or quality control in the laboratory. In-line methods of sample presentation that place the optical probe directly into the flowing grain stream may improve instrument precision (Long et al., 2008). Hyperspectral sensors (ProSpectra™ Grain Quality Analyzer, DSquared Development, LaGrande, OR, USA) may also improve precision by providing greater spectral resolution than multispectral sensors.

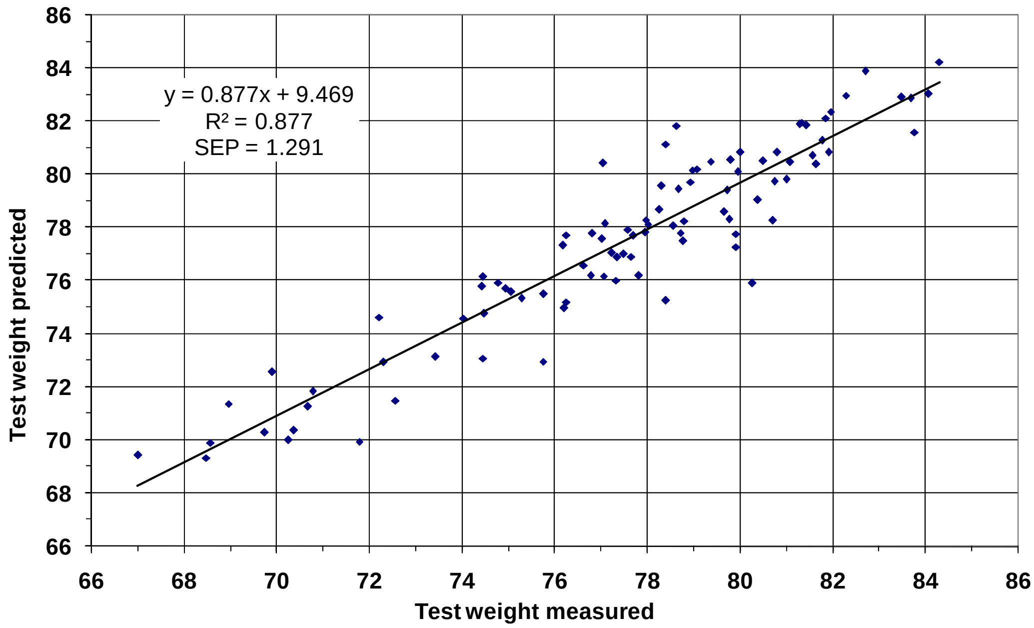

Figure 2. Correlations between measured test weight by common procedure (weighting 250 ml of grains) and predicted test weight by Zeltex AccuHarvest. n=94.

Dowell et al. (2006) found test weight to be highly correlated with NIR spectra of spring wheat ($R^2 > 0.7$) even when the covariance from grain protein concentration was statistically removed. However, a direct relationship between starch and test weight may explain the correlation between NIR spectra and protein. Starch is a major constituent of grain that has strong and broad absorption bands throughout the NIR region (Williams, 2001). Starch formation occurs in the later stages of kernel development and it is starch that gives plumpness to the kernel (Shollenberger and Kyle, 1927). Drought conditions that arrest development of the kernel and shorten the period of grain fill will produce kernels of low test weight with relatively greater protein content. The opposite will be true for grain grown under abundant moisture (i.e. high test weight with lower protein content).

On-Combine Mapping of Test Weight

The measurement accuracies reported above; however, are sufficiently promising to suggest NIR spectroscopy for use as a rough screening tool, which has implications for on-combine mapping of test weight. In semiarid environments, variation in test weight is often associated with changes in plant water availability. Therefore, test weight maps would provide post-harvest information that would aid in the interpretation of grain yield and grain protein maps. Sequential maps of test weight would help growers identify areas of consistently low or high crop productivity.

The AccuHarvest calibration model that had been developed in the laboratory was updated with new temperature coefficients as needed to adjust for warmer ambient temperatures found in the field under actual harvesting conditions. Near infrared spectra were acquired with the AccuHarvest mounted to the clean grain elevator of a JD 9600 combine. At the same time, grain samples were collected from the combine's grain bin filling auger during harvest of nine production fields. These samples were used to validate the updated prediction model. To join the spectra and grain samples in space, the geostatistical procedure of kriging was used to interpolate each data set to the nodes (n = 5012) of a common estimation grid.

Validation results, developed from use of the 5012 spectral and reference data points, were modest, with prediction statistics of R^2 = 0.66 and SEP = 1.1 kg hL^{-1} (Fig. 3). The diminished correlation is likely an outcome of sampling error, since the validation procedure was based on interpolated data. The sensor took about 60 readings ha^{-1} and thus the intensively sampled test weight data could be interpolated to produce a detailed contour map (Fig. 4). For example, fields 44E and 46E exhibited wide variation in test weight, which ranged from 71 kg hL^{-1} to 82 kg hL^{-1}, which is meaningful for wheat grain quality and its value (Bonfil et al., 2004). We observed the test weight of grain to be greater in lower, wetter slope positions than in higher, drier slope positions.

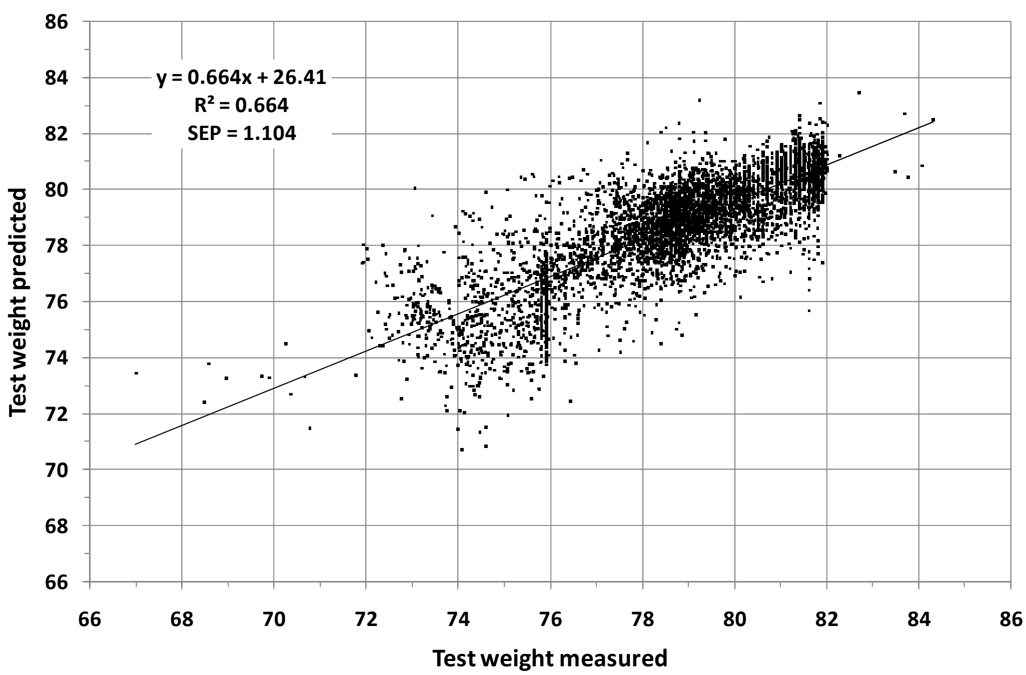

Figure 3. Correlation between interpolated measured test weight and predicted test weight by Zeltex AccuHarvest in nine fields by means of the updated calibration.

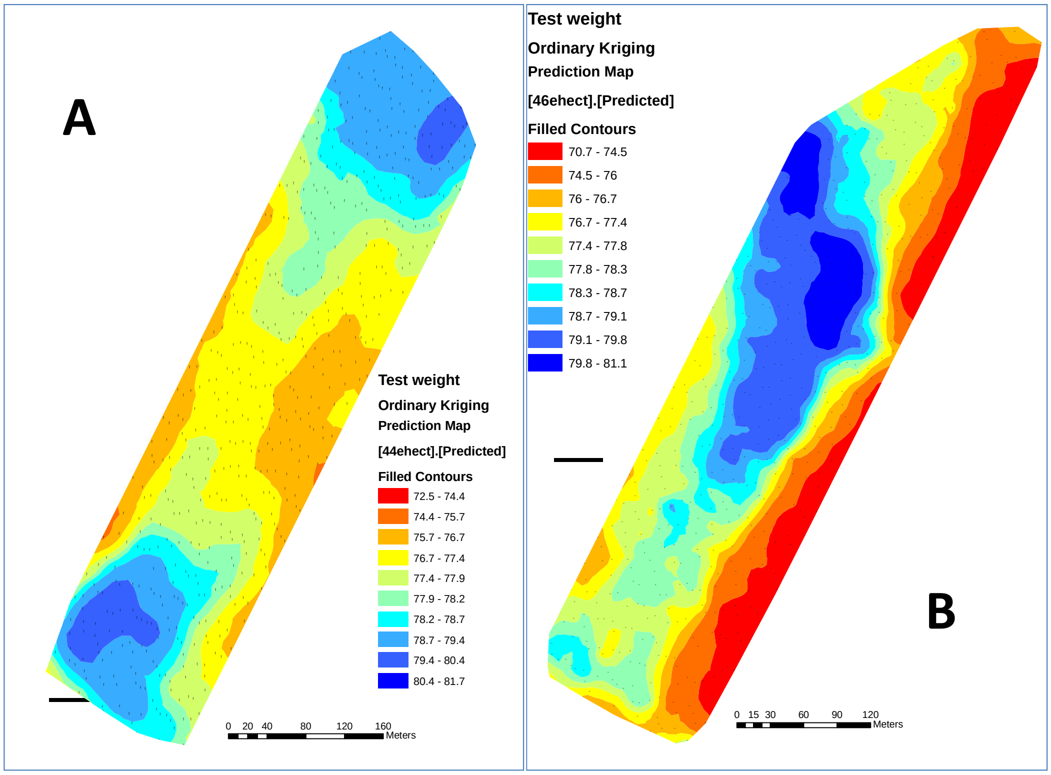

Figure 4. Prediction test weight maps as measured by Zeltex AccuHarvest in fields A- 44E and B- 46E by the updated calibration.

SUMMARY AND CONCLUSIONS

Reflectance/transmission spectra from grain can be used to predict test weight with accuracies that are suitable for rough screening, but not process control. A useful application of this technology will be on-combine mapping. Maps of test weight would provide additional, post-harvest information on grain quality that can improve a grower's ability to interpret yield maps and other spatial patterns of crop productivity within fields. Further evaluation of NIR spectroscopy is needed to fully establish performance of the method.

ACKNOWLEDGMENTS

This research was supported by Research Grant Award No. IS-3721-05R from BARD, The United States - Israel Binational Agricultural Research and Development Fund; and by the ICA (Jewish Colonization Association) foundation.

REFERENCES

Bonfil, D.J., I. Mufradi, and S. Asido. 2004. Decision support system for improving wheat quality in semi-arid regions. CD-ROM 7th International Conference on Precision Agriculture and Other Precision Resources Management. ASA-CSSA-SSSA, Madison, WI.

Delwiche, S.R. 2004. Analysis of small grain crops. p. 269-320. *In* Roberts C.A., J. Workman Jr. and J.B. Reeves III, (ed.), Near-Infrared Spectroscopy in Agriculture. ASA/CSSA/SSSA, Madison, Wi.

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 Chem. 83:529-536.

Long, D.S., R.E. Engel, and F.M. Carpenter. 2005. On-combine sensing and mapping of wheat protein concentration. Crop management. Available at http://www.plantmanagementnetwork.org/pub/cm/research/2005/protein/; verified 21 Sept. 2007.

Long, D.S., and T. Rosenthal. 2005. Evaluation of an on-combine wheat protein analyzer on Montana hard red spring wheat. p. 385–392. *In* Stafford J. et al. (ed.), Proc. 5th European Conf. Prec. Agric., Uppsala, Sweden. 9–12 June. Wageningen Academic Publ., Wageningen.

Long, D.S., R.E. Engel, and M.C. Siemens. 2008. Measuring grain protein concentration with in-line near infrared reflectance spectroscopy. Agron. J. 100:247-252.

Shollenberger, J.H., and C.F. Kyle. 1927. Correlation of kernel texture, test weight per bushel, and protein content of hard red spring wheat. J. Agr. Res. 35:1137-1152.

Williams, P.C., and K.H. Norris. 1987. Qualitative applications of near infrared reflectance spectroscopy. p. 241–246. *In* Williams P. and K. Norris (ed.), Near-Infrared Technology in the Agricultural and Food Industries. Am. Assoc. of Cereal Chemists, St. Paul, MN.

Williams, P. C. 2001. Implementation of near-infrared reflectance technology. p. 145-169. *In* Williams P. and K. Norris (ed.), Near-infrared Technology in the Agricultural and Food Industries. AACC International: St. Paul, MN.