NOTE

Triticale Moisture and Protein Content Prediction by Near-Infrared Spectroscopy (NIRS)

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ABSTRACT

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The use of near-infrared spectroscopy (NIRS) for the prediction of whole-grain triticale moisture and protein content was evaluated. Because triticale is genetically close to wheat, commercially available wheat prediction models for Foss Infratec analyzers were applied in a year-by-year basis to triticale samples harvested in Iowa between 2002 and 2006. Wheat models were not applicable to moisture prediction (SEP_{avg} = 0.37% pt; expected SEP on wheat samples 0.15% pt), but usable for screening for protein (SEP_{avg} = 0.38% pt; expected SEP on wheat samples 0.25% pt). Dedicated triticale calibrations were developed from 2002 to 2005 data. Prediction results for 2006 samples only were compared. Triticale calibrations performed better than wheat calibrations for 2006 samples (moisture $SEP_{triticale}$ = 0.29% pt, SEP_{wheat} = 0.50% pt; protein $SEP_{triticale}$ = 0.30% pt, SEP_{wheat} = 0.68% pt).

Triticale (*xTriticosecale* Wittmack), a species resulting from the intergeneric crossing of wheat and rye, has the potential to introduce valuable economic and environmental benefits to grain production systems. Since the introduction of commercial cultivars in 1969 (Zillinsky 1974), worldwide production of triticale has increased steadily to a level of 3,470,000 hectares in 2002 (Jessop 2003). The 240,000 hectares planted in the United States in 2002 were almost exclusively used for forage. However, it is becoming increasingly important as a grain crop in several parts of the world, most notably Australia and Europe.

Agronomic and utilization studies have suggested that triticale could have a wider role in North American cropping and livestock systems. Protein content and amino acid balance are in the range of wheat and rye in similar production environments (Varughese 1996) and it has greater lysine content than corn. The higher lysine content gives triticale an average of 6% greater feed value than corn (Bruckner et al 1998). It is an excellent replacement for corn as animal feed (Hale and Utley 1985; Coffey and Gerrits 1988; Myer et al 1990).

Triticale has greater vigor and grain yield than either of its parent species when grown in the same environment (Varughese 1996; Baenziger et al 2004). Like other small grains, triticale may provide yield boosts to other crops in a rotation (Zhang et al 1996); may capture residual nitrogen before it is lost (Schwarte et al 2006; Gibson et al 2007); and may provide soil erosion protection during the vulnerable late fall and early spring periods (Renard et al 1997).

Efficient utilization and trading of triticale requires rapid determination of its end-use properties, such as moisture and protein content. The use of near-infrared spectroscopy (NIRS) for the characterization of agricultural products has gained widespread use because it is fast, easy, accurate, and does not produce hazardous waste. The NIRS method has been approved by AACC International (2000) for determination of protein content of whole-grain wheat (Approved Method 39-25).

Because triticale grain possesses properties similar to wheat, we hypothesized that NIRS could accurately and rapidly determine protein and moisture content for triticale, either with the use of existing wheat prediction models or with new dedicated triticale calibrations.

MATERIALS AND METHODS

Samples

Triticale samples used in this study were harvested from 2002 to 2006 variety trials at several Iowa locations. Both winter and spring lines were grown in 2002, 2003, and 2004. Crop years 2005 and 2006 included only winter lines. This resulted in 412 samples for moisture content and 502 for protein content analysis selected from 2,994 samples (17.4% spring lines, 82.6% winter lines) resulting from the planting trials. Samples were selected on protein content using commercially available neural-network-based wheat moisture and protein calibrations (Foss North America, Eden Prairie, MN; product model WBMO0024 for moisture and WBPR0028 for protein) to obtain a uniform distribution within each crop year. No moisture measurements were performed on samples collected in 2002. Reference data statistics of selected samples are provided in Table I. Moisture content was determined in an air oven according to Approved Method 44-15A and protein content (combustion nitrogen) according to Approved Method 46-30 (AACC International 2000) using a Leco CHN-2000 analyzer. To obtain the protein content from the combustion analyzer, the nitrogen value was multiplied by 5.7, as done for wheat. The oven moisture of the ground material was also determined immediately before Leco analysis; this moisture content was used to convert the protein percentage to a constant 12% moisture basis.

Spectral Acquisition

Near-infrared spectra were acquired by a Foss Infratec analyzer 1241 (Foss North America, Eden Prairie, MN). This transmittance instrument has a spectral range of 850–1,048 nm at 2-nm increments. An 18-mm pathlength was used.

Data Analysis

Prediction models were developed using partial least squares regression (PLS-R). Calibration performances were evaluated in terms of precision, accuracy, and model fit. Standard error of prediction (SEP) or standard deviation of differences and standard error of cross validation (SECV) were used to evaluate the precision. The accuracy was determined by the bias (average of differences) and the fit of the model by the coefficient of determination

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(r^2). Calculations were realized on MATLAB v.7.0.4 (The MathWorks, Natick, MA) with the PLS_Toolbox v.3.5.4 (Eigenvector Research, Wenatchee, WA). Wheat calibrations used in this study were the same as those used to select calibration samples. These models are commercially available and are used in the official United States Department of Agriculture (USDA) grain inspection program. The product model names were WBMO0024 for moisture and WBPR0028 for protein. They were developed by an artificial neural network in a range of 6–30% for moisture and 6.9–21.8% for protein at a 12% moisture basis. These models have an expected SEP of 0.15% pt for moisture and 0.25% pt for protein (A. Gell, Foss North America, *personal communication*).

RESULTS

Prediction of Triticale Moisture and Protein with Wheat Models

The wheat calibrations were applied to spectra of the different crop years (Table I). For moisture, the wheat calibration did not give precise results. While the results from the first year (2003) were acceptable (SEP = 0.19% pt vs. an expected SEP on wheat of 0.15% pt), the effectiveness of the calibration was limited for 2004, 2005, and 2006 (SEP of 0.42, 0.37, and 0.50% pt, respectively). On the contrary, the wheat model for the protein prediction performed well for 2004 and 2005 (SEP = 0.22 and 0.24% pt) but not in the other years (SEP_{2002} = 0.36% pt, SEP_{2003} = 0.40% pt, and SEP_{2006} = 0.68% pt vs. an expected SEP on wheat of 0.25% pt). In terms of accuracy, both models performed poorly (average bias of –0.72% pt for moisture and +1.00% pt for protein). Thus the use of wheat calibrations for triticale moisture and protein prediction was not successful except for protein in 2004 and 2005. Dedicated prediction models for this cereal could offer better accuracy and precision.

Triticale Models for Moisture and Protein Prediction

Two types of models were developed. The first method included samples from all years in the calibration set and the validation was done by cross-validation leave-one-out and withholding of 25% of the calibration set as an independent validation set. The second method considered samples from 2006 as the validation year. In terms of data treatment, the moisture prediction model used autoscaling (transform all spectra to mean zero and unit variance) and the protein calibration was developed with 2nd derivative (15-pt window). Results are presented in Table II.

As expected, cross-validation results for moisture content were over-optimistic when compared with a validation procedure based on independent samples (SECV = 0.15 % pt vs. SEP = 0.29% pt). However, the precision of the protein content model for the prediction of year 2006 samples was slightly better than cross-validation results (SECV = 0.34% pt vs. SEP = 0.30% pt).

The comparison between wheat and triticale models for the prediction of the crop year 2006 showed that dedicated triticale models for protein content were better than wheat models for the prediction of 2006 samples ($SEP_{triticale}$ = 0.30% pt vs. SEP_{wheat} = 0.68% pt). However, the yearly variability created situations where the wheat models performed accurately for protein (2004 and 2005). For the prediction of the triticale moisture content, the development of a dedicated prediction model was beneficial when predicting 2006 samples ($SEP_{triticale}$ = 0.29% pt vs. SEP_{wheat} = 0.50% pt). Overall, the dedicated models were more likely to predict the next crop year's samples accurately.

DISCUSSION

In this study, we faced a problem that is inherent to the measurement of products that undergo variability in crop genetic and production environment. These variables affect the functioning of analytical techniques. Triticale samples were not genetically similar from one year to the next, and the environmental conditions varied considerably with production year (2003 and 2006 were very dry, whereas 2004 was extremely damp and humid). Those elements were most likely responsible for the results we obtained in this study. The development of specific triticale calibrations was justified. However, the variability across crop years (genetic and environmental) was likely responsible for the lower performance of the triticale prediction models compared with expectations with wheat samples and models.

TABLE I
Statistics for Triticale Moisture and Protein and Their Predictions by Wheat Artificial Neural Network Calibrations

	Moisture					Protein (12% mb)					
Parameters	2003	2004	2005	2006	Avg	2002	2003	2004	2005	2006	Avg
Sample statistics	n = 118	n = 94	n = 98	n = 268		n = 126	n = 93	n = 94	n = 98	n = 93	
					–						–
Min (% pt)	10.62	9.51	8.94	11.63	–	9.96	8.28	9.89	11.04	9.29	–
Max (% pt)	13.55	11.45	10.71	14.72	–	17.91	20.89	16.43	16.25	14.50	–
Mean (% pt)	11.59	10.40	9.80	12.61	–	12.84	13.16	12.89	13.48	11.32	–
SD (% pt)	0.50	0.49	0.35	0.68	–	1.83	2.12	1.67	1.18	1.06	–
Prediction results											
SEP (% pt)[a]	0.19	0.41	0.37	0.50	0.37	0.36	0.39	0.22	0.24	0.68	0.38
Bias (% pt)	–0.49	–1.12	–0.59	–0.68	–0.72	–0.61	–1.23	–1.01	–1.31	–0.82	1.00
R^2	0.87	0.37	0.06	0.47	0.44	0.96	0.98	0.98	0.96	0.61	0.90

[a] Standard error of prediction.

TABLE II
Triticale Calibrations with 2006 Samples Either Part or Not Part of the Calibration Set

	Moisture			Protein		
Validation Techniques	SECV/SEP (% pt)[a]	Bias (% pt)	R^2	SECV/SEP (% pt)[a]	Bias (% pt)	R^2
Leave-one-out	0.15	0.00	0.98	0.34	0.00	0.96
25% of the calibration set	0.16	0.01	0.98	0.32	–0.06	0.96
2006 samples	0.29	0.07	0.82	0.30	–0.52	0.92

[a] Standard error of cross-validation (SECV) was used to evaluate the precision of the calibration model for leave-one-out and 25% of the calibration set validation techniques (samples from 2006 are part of the calibration set). Standard error of prediction (SEP) was used for the validation using independent samples (2006 samples were used for validation and were not part of the calibration set).

CONCLUSIONS

The results of this study demonstrated that the use of dedicated models is preferred for determination of triticale moisture and protein content. The triticale protein model gave reasonable results that make the calibration usable for screening but the moisture model could be improved to reach commercial standards (0.10–0.20% pt). Another approach might be to add the triticale spectral data to the wheat prediction models to develop more robust calibrations, which would then utilize wheat historical databases.

LITERATURE CITED

AACC International. 2000. Approved Methods of the American Association of Cereal Chemists, 10th Ed. Methods 39-25, 44-15A, 46-30. The Association: St. Paul, MN.

Baenziger, P. S., Beecher, B., and Baltensperger, D. D. 2004. Improving wheat varieties for Nebraska. 2003 State breeding and quality evaluation report. Report to the Nebraska wheat development, utilization, and marketing board. University of Nebraska Lincoln: Lincoln, NE.

Bruckner, P. L., Cash, S. D., and Lee, R. D. 1998. Nitrogen effects on triticale grain yield, amino acid composition, and feed nutritional quality for swine. J. Prod. Agric. 11:180-184.

Coffey, M. T., and Gerrits, W. J. 1988. Digestibility and feeding value of B585 triticale for swine. J. Anim. Sci. 66:2728-2735.

Gibson, L. R., Nance, C. D., and Karlen, D. L. 2007. Winter triticale response to nitrogen fertilization when grown after corn or soybean. Agron. J. 99:49-58.

Hale, O. M., and Ultey, P. R. 1985. Value of Beagle 82 triticale as a substitute for corn and soybean meal in the diet of pigs. J. Anim. Sci. 60:1272-1279.

Jessop, R. 2003. World triticale area. Triticale Topics International Ed. International Triticale Association: Armidale, NSW, Australia.

Myer, R. O., Combs, G. E., and Barnett, R. D. 1990. Evaluation of three triticale cultivars as potential feed grains for swine. Soil Crop Sci. Soc. Fla. Proc. 49:155-158.

Renard, K. G., Foster, G. R., Weesies, G. A., McCool, D. K., and Yoder D. C. 1997. Predicting soil erosion by water: A guide to conservation planning with the Revised Universal Soil Loss Equation (RUSLE). U.S. Department of Agriculture. Agriculture Handbook No. 703.404. USDA: Washington, DC.

Schwarte, A. J., Gibson, L. R., Karlen, D. L., Liebman, M., and Jannink, J.-L. 2005. Planting date effects on winter triticale dry matter and nitrogen accumulation. Agron. J. 97:1333-1341.

Varughese, G., Pfeiffer, W. H., and Pena, R. J. 1996. Triticale: A successful alternative crop (Part 1). Cereal Foods World 41:474-482.

Zhang, J., Hamill, A. S., and Weaver, S. E. 1996. Corn yield after ten years of different cropping sequences and weed management practices. Can. J. Plant Sci. 76:795-797.

Zillinsky, F. J. 1974. The development of triticale. Adv. Agron. 26:315-348.

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