Near-Infrared Reflectance Spectra of Hard Red Winter Wheats Varying Widely in Protein Content and Breadmaking Potential[1]

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ABSTRACT

Near-infrared (NIR) reflectance spectra were determined on 173 hard red winter wheat flour samples. The flours included two groups of samples: 51 milled from six wheat selections and cultivars grown at one location for 11 years and 97 varietal and 25 station composites. The samples were selected to obtain a wide range in flour protein content (7.9–20.7%) and breadmaking quality. The correlation coefficient between protein content and loaf volume was only 0.308 because of the large variation in protein quality. Water absorption ranged from 48.0 to 76.0%, mixing time from 0.75 to 9.50 min, and loaf volume of bread baked from 100 g of flour from 568 to 1,328 cm^3. The logs of 1/R reflectance calibrations were derived using a Technicon 500 scanning spectrophotometer in the range 1,100-2,400 nm. The data were correlated with protein content, water absorption, dough mixing time, and loaf volume. The linear multiple correlation coefficients between NIR reflectance at 1,870, 2,052, and 2,304 nm and water absorption were 0.898 and 0.932 in calibration and prediction samples, respectively; the standard error of estimate (SEE) was 1.8%. The linear multiple correlation coefficients between NIR reflectance at 1,604, 1,632, and 1,884 nm and log mixing time were 0.848 and 0.795 for the calibration and prediction samples, respectively, and SEE 0.12 (equivalent to 1.3 min). The linear multiple correlation coefficients between NIR reflectance at 1,506, 1,534, and 1,618 nm and loaf volume were 0.896 and 0.849 for the calibration and prediction samples, respectively, and SEE was 48 cm^3. The correlation coefficient increased from 0.308 to 0.896 for the relation between protein and loaf volume or specific loaf volume, respectively, reflecting the ability of NIR to measure protein quality for breadmaking independently of protein quantity. There were differences in NIR reflectance calibration wavelengths responsible for breadmaking parameters in various groups of populations. This indicated a potential for using the spectra in varietal identification.

A relatively simple near-infrared (NIR) reflectance photometer has been shown useful in routine determinations of wheat moisture, protein, texture, grinding resistance, and starch damage (Osborne et al 1982, Osborne 1984) but not breadmaking potential (Starr et al 1981, 1983). Osborne (1984) studied a number of U.K. wheat samples using a monochromator system to measure reflectance data between 1,100 and 2,500 nm. The data correlated with protein content but not with sodium dodecyl sulfate sedimentation value, which was used as a measure of protein quality. It was concluded that NIR reflectance spectroscopy cannot provide a measure of bread-baking quality of wheat beyond that which may be predicted from protein content. A similar conclusion was reached by Downey and Dwyer (1985) and Bean and Miller (1986).

Theoretical aspects of determining strength in wheat flour by a spectral reconstruction technique were described by Wetzel and Kemeny (1986). Spies and Norris (1983) reported on the use of NIR spectroscopy of flour-water doughs to predict mixing time. A strong correlation with optimum mixing time was obtained using a combination of log 1/R and first derivative log 1/R terms. The log 1/R terms appeared to measure the amount of air incorporated into a dough, and the first derivative terms were related to the concentrations of various flour components.

Williams (1986) selected hard red spring wheat samples, which represented a minimal range in protein content and wheat hardness and a maximal range in dough mixing stability and loaf volume. Correlation coefficients with NIR reflectance spectra were 0.85 and 0.92, respectively. Standard errors of performance were 3.8 min for mixing time (for a 3.5–31 min range) and 26 cm^3 for loaf volume (for a 730 to over 1,100 cm^3 range). He confirmed results, in part, for soft white spring and winter wheats. The accuracy was considered adequate for early generation screening in wheat breeding programs.

Our studies included 173 hard red winter wheat samples covering a very wide range in protein contents, water absorption, mixing time, and loaf volume. To differentiate between the effects of protein content and protein quality, the results were expressed on an as-is protein basis and on a constant protein basis.

MATERIALS AND METHODS

Wheat and Flour Samples

The 173 flour samples were comprised of two groups: Group A totaled 51 samples representing six hard red winter wheat selections and cultivars grown in Manhattan, KS, during 1972–1974, and 1976–1983 (total of 11 crop years). Included were:

Qvivira/Tenmarq/Marquillo/Oro, C.I. No. 12995
Shawnee, C.I. No. 14157
Concho/2* Triumph, KS 644
Chiefkan/Tenmarq, KS 501097
Chiefkan/Tenmarq, KS 501099
Ottawa selection, KS 699042

C.I. 12995 and 14157 are considered cultivars (cultivated varieties). The others are selections grown for research purposes only and were never released as accented varieties. They are described in Table I.

Group B totaled 122 samples (from 1973, 1976, 1980, 1982, 1983, and 1984), of which 97 were varietal composites (from three to 31 stations), and 25 were station composites (of 4 to 15 varieties, hybrids, or selections). The locations were in the Southern Regional Performance Nursery (SRPN), the Kansas Intrastate Nursery (KIN), New York Intrastate Nursery (NYIN), and private nurseries. They are described in Table II.

The samples were described in reports of the Hard Winter Wheat Quality Laboratory by Finney et al (1972–1974, 1976–1983) and by Weipert and Pomeranz (1986). The ranges of analytical data for all 173 samples were: protein, 7.9–20.7%; water absorption, 48.0–76.0%; mixing time, 0.75–9.50 min; and loaf volume, 568–1,328 cm^3.

The straight-grade flours were obtained from an Allis-Chalmers experimental mill. The flour samples were stored at 4°C until analyzed.

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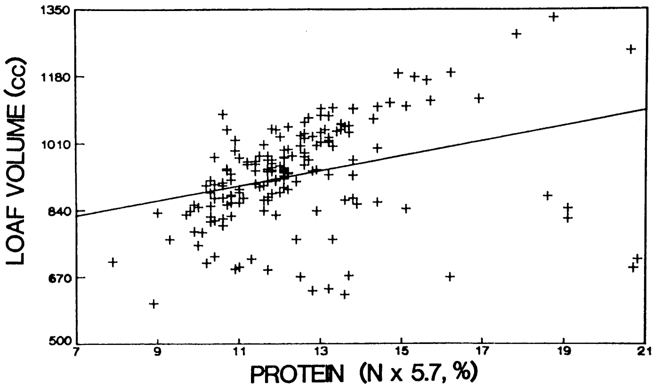

Fig. 1. Relationship between protein content (N × 5.7,%) and loaf volume (cm³), $r = 0.308$; $y = 19.118x + 692.629$.

Baking Procedure

The optimized procedure described by Finney (1984) was used for the baking tests with 100 g of flour (14% mb).

General Analytical Procedures

Protein (N × 5.7) and moisture contents were determined by AACC methods 46-12 and 44-15A, respectively (AACC 1983).

NIR Reflectance Spectra

Calibrations with the log 1/R were derived using a Technicon 500 instrument. The flour samples were presented to the instrument and light reflectance readings taken, with reference to a ceramic standard, throughout the range from 1,100 to 2,400 nm. Reflectance data on the calibration samples were searched in 4-nm steps to find the best combination of three wavelengths to measure and predict the baking parameters.

TABLE I
Parameters of Six Hard Red Winter Wheat Selections and Cultivars Grown in Manhattan, KS, for 11 Years[a]

Variety or Sel. No.	*n*	Flour Protein (%, N × 5.7)	Water Absorption (%)	Mix Time (min)	Loaf Volume (cm³)	Specific Loaf Volume (cm³/% prot.)
CI 12995	9	10.3–20.6	54.4–69.4	2.60–9.50	823–1,245	48.3–65.2
		(13.4)	(62.2)	(5.86)	(1,017)	(57.9)
CI 14157	7	9.3–18.7	52.5–69.6	3.90–7.30	765–1,328	55.4–66.8
		(12.6)	(62.9)	(5.19)	(996)	(59.2)
KS 5644	8	10.0–17.8	51.8–68.2	1.60–3.90	783–1,286	53.3–58.3
		(12.8)	(59.6)	(3.01)	(968)	(55.8)
KS 501097	10	10.2–18.6	57.4–68.2	0.90–2.80	635–929	29.3–53.6
		(13.5)	(64.3)	(1.61)	(697)	(40.2)
KS 501099	9	10.4–19.1	58.0–68.8	0.80–2.60	488–855	17.5–48.5
		(13.9)	(56.0)	(1.43)	(743)	(36.5)
KS 699042	8	10.9–20.8	52.7–64.3	0.90–2.50	625–838	21.4–45.6
		(14.9)	(50.8)	(1.46)	(699)	(31.8)

[a] Values given are ranges with averages in parentheses.

TABLE II
Range and Mean Parameters of 97 Varietal and 25 Station Composites of Hard Red Wheat Selections and Cultivars[a]

Location or Variety Composite[b]	*n*	Flour Protein (%, N × 5.7)	Water Absorption (%)	Mix Time (min)	Loaf Volume cm³	Specific Loaf Volume (cm³/% prot.)
1983 NY	6	10.7–13.8	50.4–58.7	1.9–6.0	838–1,098	50.7–64.6
		(11.9)	(56.0)	(4.2)	(936)	(57.6)
1984 NY	15	8.9–13.0	48.0–58.6	2.3–7.8	603–1,081	39.7–64.8
		(10.3)	(55.4)	(5.1)	(849)	(58.0)
1973 SRPN	5	12.1–13.8	62.2–65.8	1.1–4.6	865–1,097	44.9–61.4
		(13.1)	(63.5)	(3.0)	(933)	(52.1)
1980 SRPN	12	11.7–14.9	59.2–65.5	2.5–6.8	948–1,187	57.6–65.3
		(12.9)	(61.8)	(4.6)	(1,028)	(60.5)
1982 SRPN	9	10.6–12.6	54.4–61.2	1.8–5.3	878–964	56.0–63.7
		(11.8)	(58.3)	(3.2)	(924)	(59.3)
1983 SRPN	12	10.8–13.2	53.7–56.9	2.0–6.0	865–953	51.5–61.8
		(12.0)	(55.5)	(3.5)	(916)	(55.8)
1984 SRPN	12	10.6–12.1	54.0–60.7	2.3–7.3	885–1,084	52.9–78.7
		(11.4)	(57.4)	(3.8)	(970)	(63.5)
1983 KIN	8	10.0–11.4	56.0–59.2	3.5–6.3	847–975	55.3–69.7
		(10.6)	(57.8)	(5.0)	(912)	(62.5)
1984 KIN	8	11.2–12.6	56.4–59.7	3.6–7.9	956–1,064	59.9–67.5
		(12.0)	(57.6)	(5.3)	(1,014)	(63.5)
1983 Hybrids	4	12.1–12.7	54.4–58.1	2.9–4.3	978–1,075	59.2–65.0
		(12.4)	(55.9)	(3.9)	(1,017)	(69.2)
1983 Private nursery	6	13.8–16.9	53.6–63.2	1.6–6.5	968–1,189	51.7–60.0
		(15.0)	(59.9)	(3.8)	(1,074)	(55.0)
Station composites (SRPN)						
1973	23	7.9–15.6	69.5–69.0	3.3–7.1	708–1,178	53.6–61.1
		(12.4)	(64.4)	(4.4)	(969)	(58.0)
1976	2	11.7–13.7	63.5–68.5	4.5	978–1,055	58.8–62.2
		(12.4)	(66.0)	(4.5)	(1,017)	(60.5)

[a] Values given are ranges with averages in parentheses.
[b] SRPN = Southern Regional Performance Nursery; KIN = Kansas Intrastate Nursery.

RESULTS

The positive and strong relationship between protein and loaf volume in individual wheat cultivars is well known, with usual positive correlations better than 0.90 (Finney 1984). Similarly, it has been well established that NIR accurately measures the protein in wheat. It was important, because of these relationships, that the experimental material deviate from this normal fit of protein and loaf volume to obtain evidence that NIR was measuring loaf volume independently from the presence of protein. A plot of flour protein versus loaf volumes of the samples selected for this study (Fig. 1) deviates from the norm with a correlation of only $r = 0.308$. The low correlation resulted from the very wide range in protein quality of these experimental wheats, as also indicated by specific loaf volumes in Tables I and II.

The procedure used was to randomly split the 173 samples into two groups. The odd-numbered samples (87) were used as a calibration set and that calibration was then used to predict the baking parameters of the other half (even numbered samples, 86). The combination of the best three wavelengths from the NIR spectra (log 1/R) and the multiple linear regression equation coefficients were then used to predict the baking characteristics of loaf volume, mixing time, and water absorption of both sets.

We obtained a correlation of $r = 0.896$ with loaf volume at 1,506, 1,534, and 1,618 nm (Fig. 2) for the calibration set. When using the even-numbered samples as unknowns, the correlation dropped to $r = 0.849$. The linear relationships (slopes of the calibration and prediction lines) were, however, nearly identical.

To study further the influence that protein may have in this prediction equation, the loaf volumes were converted to "specific volume" by subtracting 250 cm^3 from the observed loaf volume and dividing by the percent protein. The value of 250 cm^3 was chosen because this has been found to be a good approximation of loaf volume with zero protein. Using the specific volume and doing the same treatment of calibrating with the odds and predicting the evens with that calibration equation, a correlation of $r = 0.817$ was found (Fig. 3). This correlation was not as strong as with observed loaf volume (0.817 vs. 0.896); however, it was still significant and indicates measurement of some parameter relating to loaf volume independent of protein. The difference between the 0.817 and 0.896 correlation coefficients possibly resulted from protein interaction in the NIR prediction of loaf volume.

The NIR spectral scans were used to investigate dough mixing time. Finney (1984) demonstrated a strong relationship between dough mixing time and loaf volume, which has found wide use as a flour quality indicator. Again, using the odd numbered samples as a calibration set, a prediction fit for mixing time gave a good correlation ($r = 0.768$) that decreased ($r = 0.679$) when the evens were run against this calibration (Fig. 4). A long observed effect of protein on mixing time demonstrates a curvilinear relationship with mixing time and loaf volume (not shown) and suggested that an improved fit with the NIR spectral data might be obtained if the mixing time were converted to log values. Results of calibration and prediction with the log of mixing time were plotted and shown in Figure 5. The prediction relationship improved to give an r value of 0.848 versus the 0.768 without the log conversion. Also, an interesting observation is that the three best wavelengths (1,604, 1,632, and 1,884 nm) were the same for both mix time and the log of mix time.

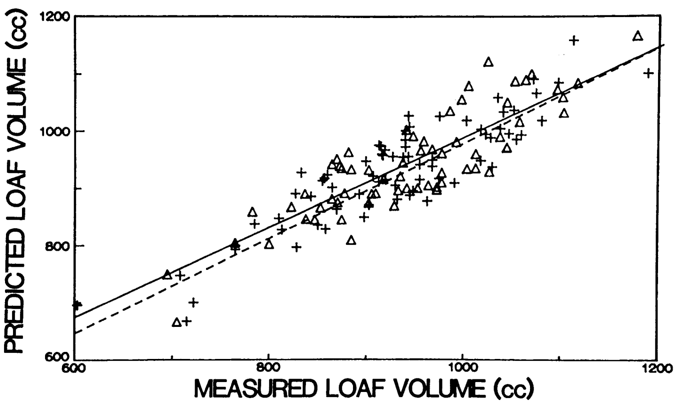

Fig. 2. Relationship betweeen measured and predicted loaf volume for odd samples (+, calibration), $r = 0.896$; $y = 183.4 + 0.803x$ (- - -), and even samples (Δ), $r = 0.849$; $y = 201.8 + 0.787x$ (——).

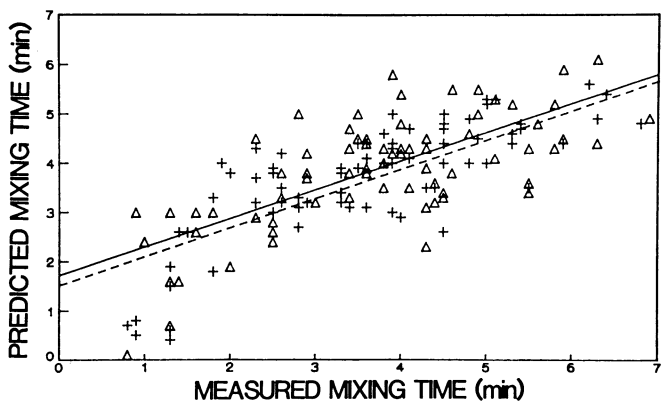

Fig. 4. Relationship between measured and predicted mixing time for odd samples (+, calibration), $r = 0.768$; $y = 1.52 + 0.59x$ (− − −), and even samples (Δ), $r = 0.679$; $y = 1.71 + 0.57x$ (——).

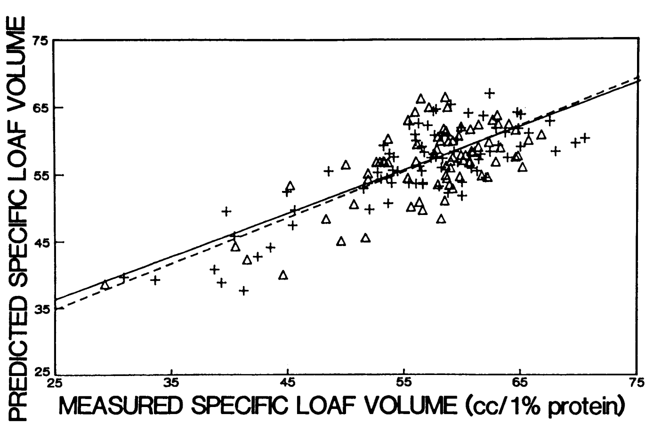

Fig. 3. Relationship between measured and predicted specific loaf volume for odd samples (+, calibration), $r = 0.817$; $y = 18.70 + 0.667x$ (− − −), and even samples (Δ), $r = 0.677$; $y = 20.45 + 0.633x$ (——).

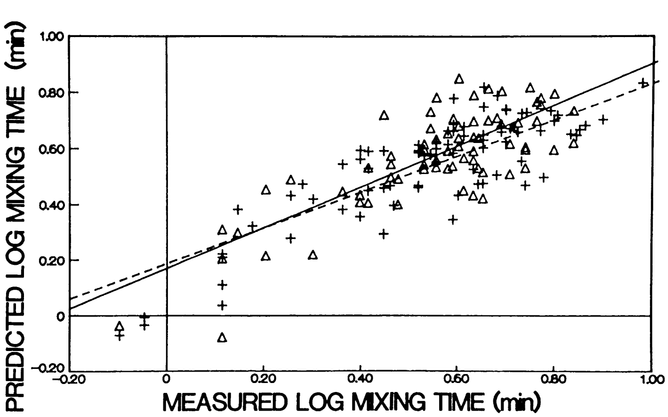

Fig. 5. Relationship between measured and predicted log mixing time for odd samples (+, calibration), $r = 0.848$; $y = 0.153 + 0.714x$ (− − −), and even samples (Δ), $r = 0.795$; $y = 0.154 + 0.743x$ (——).

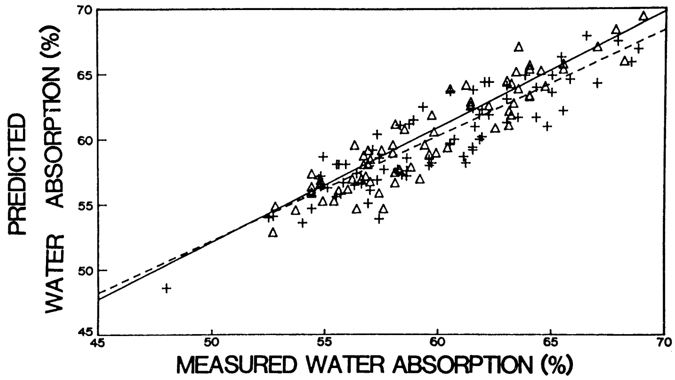

Fig. 6. Relationship between measured and predicted water absorption for odd samples (+, calibration), $r = 0.898$; $y = 11.63 + 0.806x$ (– – –), and even samples (Δ), $r = 0.932$; $y = 6.18 + 0.906x$ (——).

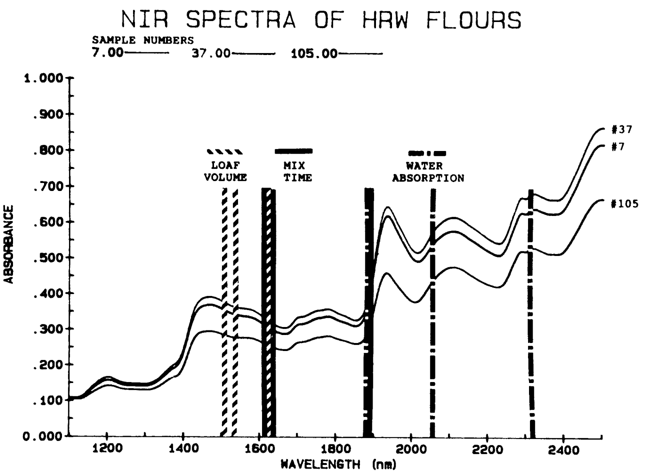

Fig. 7. Typical near-infrared spectra of three samples and wavelength ranges related to loaf volume, mixing time, and water absorption of wheat flours.

TABLE III
Summary of Three Best Wavelengths (λ), *t* Values, *F* Values, Multiple Correlation Coefficients (*r*), and Standard Errors of Estimate (SEE) for Three Important Quality Parameters

Baking Parameters	λ	*t*	*F*	*r*	SEE
Loaf volume, cm^3	1,506	−12.9	···	···	···
(603–1,189)	1,534	13.9	90.8	0.90	48
	1,618	−16.0	···	···	···
Log mix time, min	1,604	12.0	···	···	···
(−0.097 to 0.978)	1,632	−12.3	63.9	0.85	0.12
	1,884	12.7	···	···	···
Absorption, %	1,870	−12.6	···	···	···
(48–68.8%)	2,052	14.0	99.0	0.90	1.8
	2,304	−14.1	···	···	···

Water absorption is another important characteristic of baking quality and was investigated in the same manner. Water absorption, like loaf volume, was highly correlated with the log 1/R spectral data (Fig. 6) and gave $r = 0.898$ with the combination of the best three wavelengths. Unlike loaf volume and mixing time, where there was a slight loss in the predictive fit when running the even-numbered samples against the calibration equations derived with the odd-numbered samples, the fit with water absorption actually increased to $r = 0.932$ when predicting the water absorption of the even numbered samples.

The active and interactive wavelengths found useful to characterize hard red winter wheat flour for protein content, loaf volume, mixing time, and water absorption are identified on spectrum plots of three samples that showed a range of absorbance in Figure 7. A summary of the wavelengths (λ), their statistical *t* values, *F* ratios, *r* values, and standard errors of estimate (SEE) is given in Table III. Wavelengths 1,534 nm and 2,052 nm were established to relate to protein and 2,304 nm to lipids.

DISCUSSION

The correlation coefficients were as high within the first group of 51 samples (6 varieties from 11 years) as in the total population. When the samples from the first group were used to predict breadmaking potential of the second group (varietal and location composites), different significant wavelengths were obtained, and the correlation coefficients were low. The results point to variety-specific effects on NIR spectra and to the possibility of using those spectra for variety identification, as suggested by Bertrand et al (1985).

The results could be improved by adjustment on a year-to-year basis. When predicted results were examined on a year-to-year basis, in some years all points were consistently above or below the calibration regression line. This is in agreement with the year-to-year effects often observed in routine calibration for protein content.

The use of first and second derivatives of log 1/R did not improve the correlations. Similarly, the addition of a fourth wavelength for prediction of loaf volume provided no improvement. Finally, selection of NIR reflectance spectra to predict crumb grain did not yield satisfactory results. The difficulty lies, in part at least, in the nonlinear scale of crumb grain and texture and the fact that sensory parameters are affected by loaf volume. The latter, in turn, is affected (to varying degrees) by protein content. Whereas loaf volume can be expressed on a common protein basis, such an expression cannot be done in a meaningful way for crumb grain and texture.

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