Changes in Maturing Wheat as Determined by Near-Infrared Reflectance Spectroscopy

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ABSTRACT

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Kernels of nine wheat varieties grown in 1986 in Kansas were harvested at 11 stages of maturity and kernels of seven wheat varieties grown in the state of Washington at nine stages of maturity (7–42 days after flowering). The wheats were freeze-dried, ground, equilibrated to about 12% moisture, and evaluated by near-infrared reflectance spectroscopy throughout the range of 1,100–2,400 nm at 4-nm steps. Peaks in four spectral regions were present in immature wheat and absent in mature wheat, and one peak was found in mature wheat only. The most consistant and conspicuous peak, which decreased gradually during maturation, was at 2,276–2,288 nm; it is probably associated with a nonstarchy polysaccharide.

Near-infrared reflectance (NIR) spectroscopy has found wide application in determination of gross (major) components of agricultural products, by-products, and foods (Osborne and Fear 1986, Hollo et al 1987, Williams and Norris 1987). NIR spectroscopy is finding increasing application in following changes which take place during the processing of agricultural raw materials and production of foods as well as in continuous quality control. We report here on spectral changes that take place in maturing wheat. The usefulness of the technique to determine the presence of immature wheat in a commercial grist is explored.

MATERIALS AND METHODS

Kernels of nine hard red winter (HRW) wheat varieties grown in 1986 in Manhattan, KS, were harvested at 11 stages of maturity: 7, 10, 12, 14, 17, 19, 21, 24, 28, 35, and 42 days after half the kernels on a head were flowering (DAF). The wheats from Kansas were combine ripe at 24–35 DAF. The HRW varieties included: Arkan, Bounty 201, Bounty 205, Brule, Centurk, Hawk, Newton, TAM 107, and TAM 108. The following seven wheat varieties were grown in 1986 in Pullman, WA: soft white winter Brevor, Nugaines, Stephens, and Vakka; club Tres; and hard red winter Kharkoff and Wanser. They were harvested at nine stages of maturity; the Washington wheats were combine ripe at 40 to 44 DAF. Ten to 12 heads (from each variety at each maturity stage) were freeze-dried and hand threshed.

The cleaned samples were ground on a Wiley micromill to pass a 20-mesh screen and were equilibrated at 26°C and 60% rh for 10 days to attain a moisture of about 12%. In addition to 1,000-kernel weight, moisture, ash, protein, and pentosans (soluble and total) were determined on the ground samples. Moisture, ash, and protein were determined according to AACC approved methods (1983). Soluble and total pentosans were determined by the method of Hashimoto et al (1987). The ground samples were examined for NIR light reflectance on a Technicon 500 spectrophotometer. Readings were taken with reference to a ceramic standard throughout the range 1,100–2,400 nm. Reflectance data were determined in 4-nm steps. To find the exact maximum absorbance of peaks, the samples were scanned in 1-nm steps. Next, the instrument software was used for data transformation, and the peak was determined (Williams and Norris 1987).

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RESULTS AND DISCUSSION

The results of 1,000-kernel weight determinations for the 11 stages of maturity of the Kansas grown wheats are summarized in Figure 1. Only maximum, minimum, and mean data are presented. Basically, there was little increase in dry matter kernel weight beyond 28 DAF. Data on some compositional characteristics of the nine HRW wheats grown in Kansas are given in Table I. Only data for 14, 21, and 35 DAF are presented. As wheat matured, kernel weight increased, protein varied slightly but inconsistently, and ash and pentosans (especially soluble pentosans) decreased. The decreases in ash and pentosans were highly correlated (Table II). For calculation of correlation coefficients, results for 72 samples were used. The results for the HRW Kansas wheats were confirmed by testing seven wheats grown in Pullman, WA. These are summarized in Table I. Note that the wheats grown in the Pacific Northwest required longer growing periods, attained higher 1,000-kernel weights, and were lower in ash and total pentosans than the wheats from Kansas.

For calculation of the NIR results in Table II, multiple correlations were computed on the basis of three wavelengths which produced the highest values. The highest multiple correlation coefficient for NIR absorbance versus total pentosan content was 0.896 for the combination 1,680, 1,688, and 1,702 nm and 0.893 for the combination of 2,234, 2,332, and 2,444 nm.

Figure 2 compares NIR reflectance spectra in Arkan and TAM 108, respectively, at three stages of maturity: 7, 24, and 35 DAF. Those results were used to calculate differences in spectra, using the 24 DAF spectrum as reference. The results are summarized in Figure 3. Similar results were obtained for the other seven

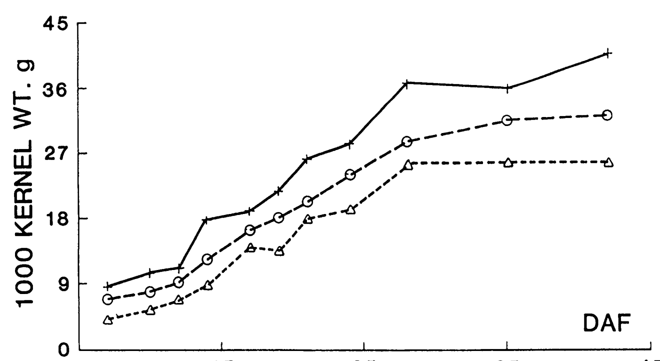

Fig. 1. Changes in 1,000-kernel weight (g) of maturing hard red winter wheats, harvested 7–42 days after flowering (**DAF**); maximum (+), minimum (△), and mean (○) data for nine cultivars.

TABLE I

Composition[a] of Kernels from Wheat Grown in Manhattan, KS, and Pullman, WA, and Harvested at Various Stages of Maturity

Kernel Weight and Component	Days After Flowering 14 Min	14 Max	14 Mean	21 Min	21 Max	21 Mean	35 Min	35 Max	35 Mean
Manhattan, KS									
1,000-Kernel wt (g)	7.53	17.73	12.20	17.99	26.15	20.36	28.17	35.93	31.52
Protein (N × 5.7, %)	10.1	12.5	11.0	8.4	10.8	9.7	9.0	11.8	10.4
Ash (%)	1.90	2.36	2.15	1.70	1.99	1.84	1.48	1.73	1.64
Soluble pentosans (%)	3.41	1.05	2.58	1.04	1.95	1.42	0.55	0.93	0.72
Total pentosans (%)	6.17	8.24	7.57	5.37	8.22	6.51	4.38	6.42	5.45
	14 Min	14 Max	14 Mean	37 Min	37 Max	37 Mean	42 Min	42 Max	42 Mean
Pullman, WA									
1,000-Kernel wt. (g)	9.65	25.29	12.97	33.61	52.61	42.90	31.72	53.61	41.79
Protein (N × 5.7, %)	10.65	13.66	11.68	10.36	13.48	11.19	10.49	12.73	11.29
Ash (%)	1.71	2.48	2.29	1.35	1.67	1.52	1.31	1.68	1.52
Soluble pentosans (%)	1.33	2.71	2.19	0.69	0.90	0.78	0.63	0.90	0.78
Total pentosans (%)	4.53	6.69	5.58	4.22	5.12	4.65	4.13	5.44	4.75

[a]14% moisture basis.

TABLE II

Correlation Coefficients Between 1,000-Kernel Weight, Ash, Soluble Pentosans, Total Pentosans, and Near-Infrared Absorbance of Kansas Wheats Harvested at Various Stages of Maturity

Kernel Weight and Component	Ash	Soluble Pentosans	Total Pentosans	Near-Infrared Absorbance
1,000-Kernel wt.	−0.875	−0.810	−0.729	0.968 (1,926, 1,954, 2,388)[a]
Ash	···	0.804	0.491	0.912 (2,262, 2,360, 2,402)
Soluble pentosans		···	0.590	0.965 (1,926 2,234, 2,248)
Total pentosans			···	0.893 (2,234, 2,332, 2,444)

[a]Values in parentheses denote wavelengths in nm.

HRW wheat varieties from Kansas (Bounty 201, Bounty 205, Brule, Centurk, Hawk, Newton, and TAM 107) and the seven wheat varieties from the state of Washington and are not reported here.

The following wavelengths, corresponding to specific components, were identified in the literature: 1,360–1,371, nm carbohydrates including glucose, sucrose, starch, cellulose and hemicellulose; 1,580–1,589 nm, the same carbohydrates; 2,110 nm, hemicellulose, and a broad starch band, $CONH_2$, CONHR; 2,273 nm, cellulose; 2,275 nm glucose; 2,276–2,278 nm starch.

Robert et al (1988) identified NIR wavelengths corresponding to proteins (1,980, 2,052, 2,180, 2,265, 2,300, and 2,345 nm),

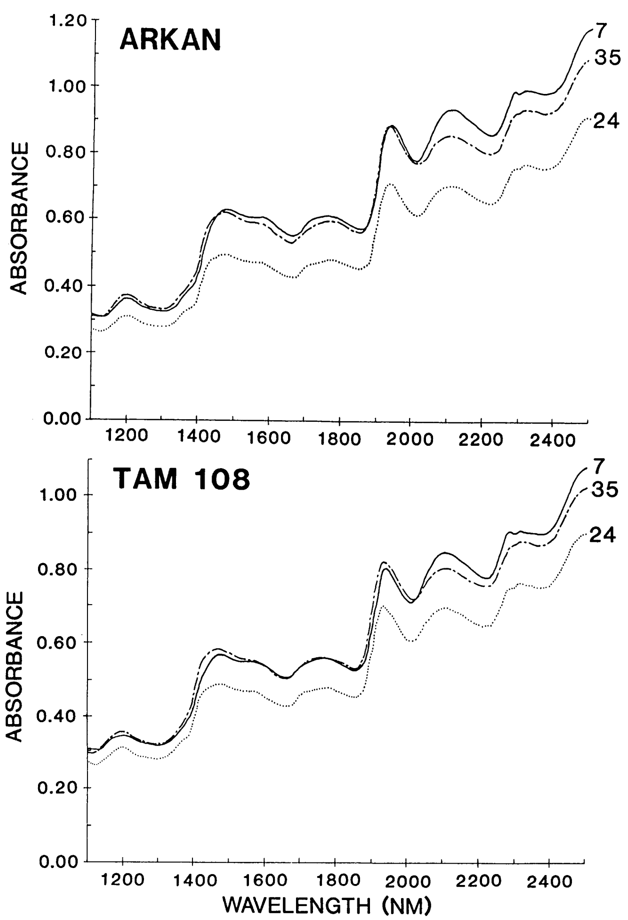

Fig. 2. Near-infrared reflectance scans (log 1/*R*) of Arkan and TAM 108 wheats harvested at 7, 24, and 35 days after flowering.

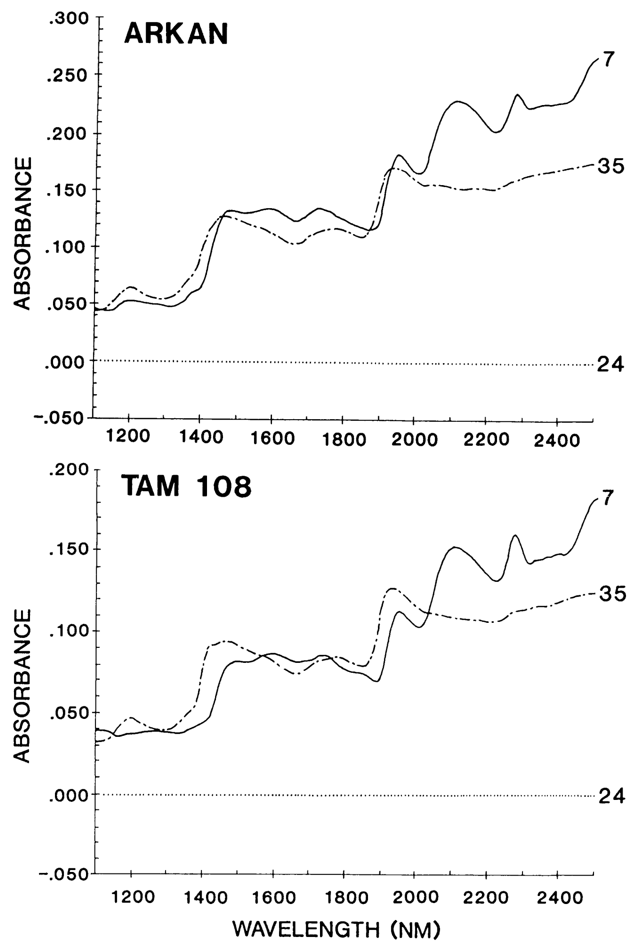

Fig. 3. Differences in near-infrared absorbance scans of Arkan and TAM 108 wheats harvested at 7, 24, and 35 days after flowering (DAF). The spectra were compared with the absorbance at 24 DAF set as base line.

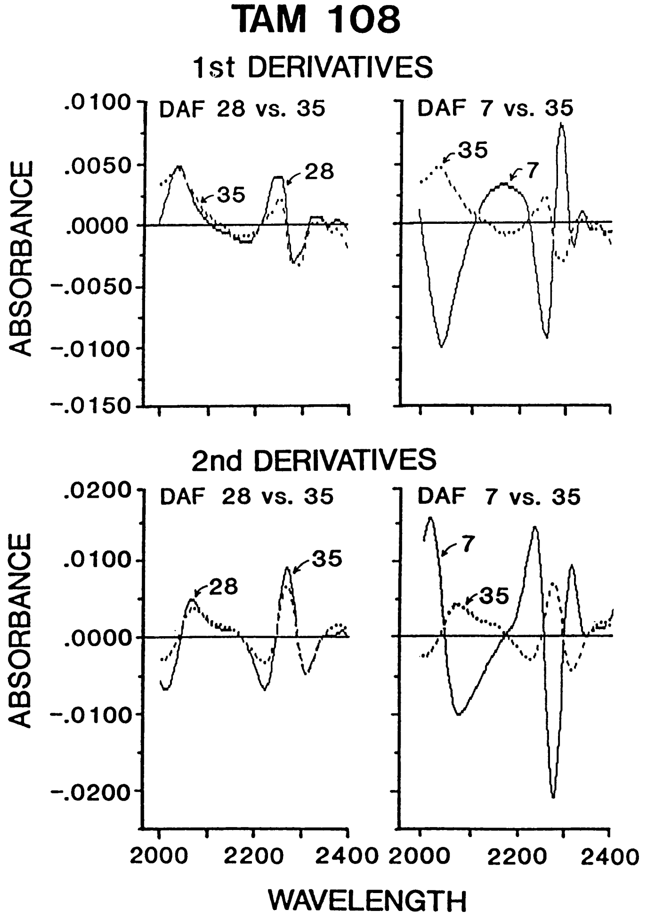

Fig. 4. First and second derivatives of the near-infrared reflectance scans of TAM 108 wheats in the 2,200–2,400 nm range. Comparisons of 28 and 35 days after flowering (**DAF**) and 7 and 35 DAF.

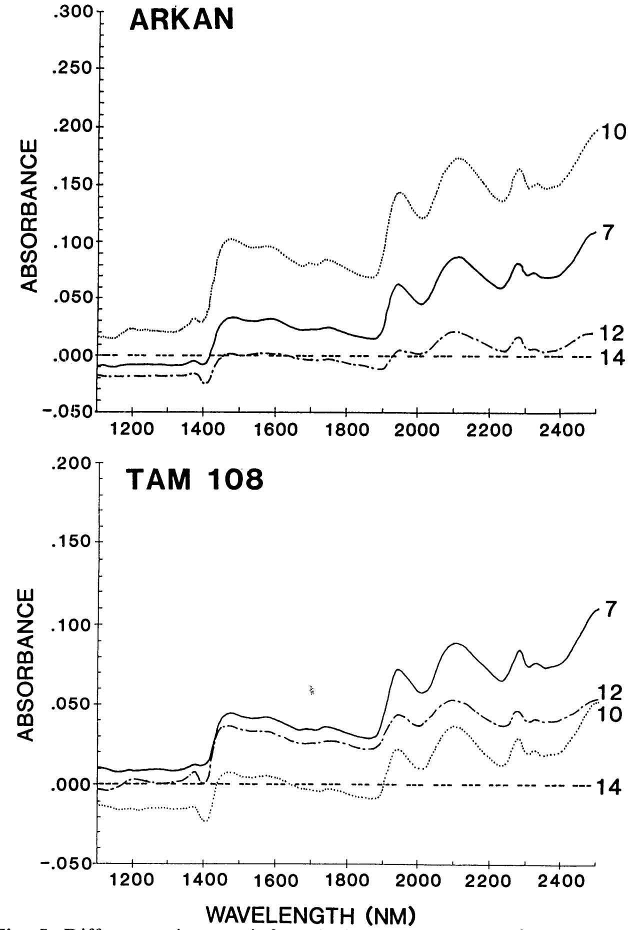

Fig. 5. Differences in near-infrared absorbance scans of Arkan wheats harvested at 7, 10, 12, and 14 days after flowering (DAF). The spectra were compared with the absorbance at 14 DAF set as base line.

cellulose (2,096, 2,284, 2,332, and 2,356 nm), starch (2,080 and 2,100 nm), and lipids (2,148 nm) in wheat and wheat flour.

Examination of Figure 3 shows consistent differences in four spectral regions: around 1,380 nm, 1,568 nm, 2,110 nm, and 2276–2288 nm. The four spectral differences (four wavelength regions) may be associated with fewer or more components. In addition, a peak at about 1,200 nm (probably starch) was present in mature wheat and absent in immature wheat. One of the consistent and conspicuous changes during maturation was disappearance of the 2,276–2,288 nm peak (probably associated with nonstarchy polysaccharides and with a decrease in soluble pentosans, Table I). The disappearance of the peak can be seen clearly in Figure 4, which shows the first and second derivatives of the NIR reflectance scans of TAM 108 wheat, in the 2,200–2,400-nm range. The derivative plots for the samples from 28 and 35 DAF are qualitatively identical. The derivative plots for the samples from 7 and 35 DAF show large peaks at 7 DAF and practically none at 35 DAF.

The disappearance of the peak was gradual, as shown in Figure 5, which compares differences in the NIR reflectance spectra of Arkan and TAM 108 harvested 7, 10, 12, and 14 days DAF. In both cultivars, compared with the NIR spectrum at 14 days, the 2,276–2,288 nm peak was strongest in the wheat at 7 DAF and generally decreased as the wheat matured.

CONCLUSIONS

The results of this study identify by NIR reflectance the presence of up to four peaks that disappear during wheat maturation. The peak at 2,276–2,288 nm seems best suited to identify immature wheat in a mixture because it is most conspicuous and consistent. In addition, its gradual disappearance during maturation makes attractive the possibility to determine the amount of immature wheat in a mixed grist. The determination can be based on the examination of the 2,276–2,288 nm peak alone or in combination with other wavelengths. Thus, for instance, when 10 mixtures (ranging from 10 to 100%, at 10% increments) of immature (7 DAF) and mature (42 DAF) Nugaines wheat were prepared, the simple correlation coefficient between the percentage of immature wheat in the mixture and reflectance at 2,276 nm was 0.992. It should be noted that similarly high simple correlation coefficients were recorded for the wavelengths 1,618 and 1,842 nm (0.991 and 0.992, respectively). A combination of the three wavelengths (2,276, 1,618, and 1,842) increased the multiple correlation with percent of immature wheat in the blend to 0.998. Studies on the absence and presence of the various compounds in maturing wheats from various classes as well as in flours milled from those wheats are underway in our laboratories.

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