Predicting a Hardness Measurement Using the Single-Kernel Characterization System

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ABSTRACT

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The single-kernel characterization system (SKCS) crushes individual kernels and uses algorithms based on the force-deformation profile data to classify wheat samples into soft, hard, or mixed market classes. Those data were utilized to produce a predictive equation for softness equivalent (SE), a direct measure of wheat kernel texture obtained from milling wheat on a modified Brabender Quadrumat Jr. mill and sieving system. Predicted SE values had a high correlation ($r^2 = 0.996$) with actual SE milling values. In contrast to SKCS hardness index values, predicted SE values accurately responded to varying kernel moisture content and kernel size, within the ranges examined. Therefore, using the SKCS data to predict an independent measure of kernel texture (e.g., SE) may be a valuable augmentation to or replacement for using SKCS algorithms to classify wheat.

The single-kernel characterization system (SKCS) model 4100 (Perten Instruments North America, Inc., Reno, NV) is designed to classify wheat into four ranges based on kernel texture (hardness or softness) characteristics. Instrumental data are expressed as mathematical algorithms that describe the crushing (force-deformation profile) of individual wheat kernels. Classification is based on the mean and distribution of various expressions of texture, size, and moisture data generated from crushing 300 wheat kernels. The SKCS is designed to isolate individual kernels, weigh them, and then crush them between a toothed rotor and progressively narrowing crescent-shaped gap. The force-deformation profile during the crushing of the kernel and the conductivity between the rotor and electrically isolated crescent are measured against time. That information is algorithmically processed to provide the weight, size, moisture, and hardness of the kernel. Processing a 300-kernel sample takes approximately 3 min. Generated reports utilize the mean values and standard deviations of individual kernel data obtained from the 300-kernel sample. Classification is based on the distribution of the data for the individual kernel measurements. Other reported data are hardness index and kernel size (diameter), moisture content, and weight. There are other "lower level instrument data" that are not reported, but can be accessed, evaluated, and used for other purposes, as reported in this study.

Hardness index values are based on algorithms that attempt to segregate wheats on a numeric scale on which hard wheats are "algorithmically forced" toward a value of 75 and soft wheats toward a value of 25. This scale is similar to that used by a near-infrared reflectance spectroscopy (NIRS) method for assessing the texture of bulk samples of wheat (AACC 1995). The NIRS method also arbitrarily assigns a value of 75 for hard and 25 for soft wheat standard samples. Although that numerical assignment is based on an arbitrary scale, it apparently works for NIRS data because wavelength scatter is a function of meal particle size after grinding, a direct expression of kernel texture. The SKCS values, being mathematical expressions of machine-generated crushing data, are not founded on a traditional, direct method (i.e., milling, grinding, energy requirement, sieving, and particle size) of measuring the texture (hardness or softness) of wheat kernels.

Investigations with a prerelease prototype of the SKCS indicated that soft wheat kernel size and moisture content (above 15%) may influence the instrument's classification result, especially for soft wheat. Increasing the moisture content of wheat kernels softens them, as has been shown using several different types of texture measurements: probe penetration (Smeets and Cleve 1956, Meppelink 1974), compression (Newton et al 1927, Katz et al 1961, Meppelink 1974, Al Saleh and Gallant 1985), work or torque to grind (Obuchowski and Bushuk 1980, Hook and Wallington 1981), time to grind (Hook and Wallington 1981; Miller et al 1981a,b; 1982), flour particle size distribution based on sieving and near-infrared spectroscopy (Miller et al 1982), and meal particle size index (Symes 1961, Meppelink 1974, Obuchowski and Bushuk 1980, Yamazaki and Donelson 1983).

Interestingly, in some cases, the work energy input required to grind or the time to grind has been observed to increase as moisture content increased. Yet, on the same samples, other methods of texture evaluation showed that those samples were definitely softer (Meppelink 1974; Obuchowski and Bushuk 1980; Hook and Wallington 1981; Miller et al 1981a, 1982). One explanation was that higher-moisture wheats clogged the burrs of the grinding apparatus or otherwise increased residence time in the grinding chamber, thereby increasing the work required to expel the ground sample (Miller et al 1981a). That phenomenon also may occur in the SKCS instrument.

The cracking strain of wheat kernels subjected to crushing was shown to decrease when kernel diameter decreased (Newton et al 1927). When smaller kernels have been produced from a given sample by sieving, they have been observed to have softer wheat kernel texture (Miller et al 1981b) and softer barley kernel texture (Blum et al 1960). Additionally, grinding resistance and particle size index have both been shown to be affected by kernel size, with smaller kernels tending to be softer (Pomeranz et al 1985).

Break flour yield is primarily a function of wheat kernel texture. Softer kernels produce more break flour. Combined with the first two or three reduction flour streams, the first two or three break flour streams are the higher-quality portion of flour milled from soft wheat and sell at a premium price. This report evaluated kernel texture as softness equivalent (SE), a value equivalent to break flour from a large mill, but determined during the milling of wheat on a smaller, modified Brabender Quadrumat Jr. mill.

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This study selected SKCS instrumental "raw data" values that were shown to predict SE. It associated the algorithmically expressed SKCS data with a practical and direct evaluation of wheat kernel texture (SE). The results suggested that other traditional measures of kernel texture (flour particle size, meal particle size index, grinding force, grinding time, NIRS, etc.) also may be predicted. The goal was to impart increased flexibility and utility to the SKCS instrument. The influence of kernel moisture content and kernel size on those data were studied. The study illustrated a difference between predicted SE values and SKCS hardness index values relative to kernel moisture content and kernel size. It also demonstrated the added utility of the predicted SE value (or other similar approach) for use as an augmentation of or alternative foundation for a SKCS classification.

MATERIALS AND METHODS

Five sets of wheats were utilized. One set was chosen to generate a predictive equation and one set was used to validate the predictive equation. Another set was used to demonstrate the influence of wheat moisture content. Two other sets demonstrated the influence of wheat kernel size.

The equation generation set consisted of 14 wheats. The cultivar, U.S. wheat class, milling SE, SKCS hardness index, SKCS grain moisture, and drying oven grain moisture contents of those wheats are shown in Table I. Greater SE values indicate softer grain texture. Smaller hardness index values indicate softer grain texture. Samples were milled (as-is moisture basis) on a modified Brabender Quadrumat Jr. mill using the procedure of Finney and Andrews (1986) modified by substituting a 40-mesh (470-μm) screen for the 54-mesh (290-μm) screen and increasing sieving time to 90 sec. Quadrumat Jr. SE is calculated as follows:

$$SE = \{[(wt - Ov40) - Ov94]/(wt - Ov40)\} \times 100 \qquad (1)$$

in which wt is starting wheat weight, Ov40 is weight over a 40-mesh (470-μm) screen, and Ov94 is weight over a 94-mesh (155-μm) screen after sieving.

The validation set consisted of the 42 wheat samples (Table II). Some of the soft wheats were selected for their lower SE values, identifying them as relatively hard soft wheats. Some of the hard wheat samples were selected for higher SE values, identifying them as relatively soft hard wheats. Other wheat samples were chosen because they were harder hard wheats or softer soft wheats. Therefore, the validation set had a large range in kernel texture and overlap in texture between the hard and soft wheat classes.

TABLE I
Cultivar, Class, Softness Equivalent, Single-Kernel Characterization System (SKCS) Hardness Index, SKCS Moisture, and Oven Moisture for the 14-Sample Prediction Set

Cultivar	Wheat Class[a]	Softness Equivalent (%)	SKCS Hardness Index	SKCS Moisture (%)	Oven Moisture (%)
Caldwell	SRW	66.8	0.5	11.9	12.0
Caldwell	SRW	62.4	3.5	12.3	12.6
Caldwell	SRW	60.3	12.9	11.6	11.9
Titan	SRW	52.5	25.2	11.3	11.4
Nugaines	SWW	47.7	38.8	11.3	11.3
Tres	SWW	45.5	33.5	10.8	10.8
Stephen	SWW	42.1	24.9	10.1	10.1
Newton	HRW	35.5	66.7	11.1	11.5
TAM 105	HRW	33.5	79.6	10.8	10.8
Bennet	HRW	32.3	74.8	11.2	11.6
Len	HRS	28.8	74.3	11.1	11.4
KSU-2180	HRW	25.8	84.6	11.1	11.6
Yecora Roja	HRS	24.1	78.4	10.8	10.6
Westbred 881	Durum	14.4	76.6	9.5	9.2

[a] SRW = soft red winter, SWW = soft white winter, HRW = hard red winter, and HRS = hard red spring.

Four soft wheats (Cardinal, Adena, Excel, and Ohio 490) were subsampled and tempered to four to six moisture contents. Tempered wheats were sealed and stored for one week before analysis. SKCS determined moisture content was used to adjust the predicted SE values to 14% moisture and to plot data.

A fourth set consisted of two soft wheats (Pioneer 2510 and LB292) and a hard spring wheat (Butte 86), each separated by sieving into subsamples that differed in 1,000-kernel weight (TKW) (Count-A-Pak, Seedboro, Chicago). There were five Pioneer 2510 subsamples, six Butte 86 subsamples, and nine LB292 subsamples. Another set consisted of three samples of Pioneer 2580 that were grown at three different locations. They were sieved on a dockage tester (model XT2, Carter-Day Co., Inc., Minneapolis, MN) to produce three subsamples of large, medium, and small kernels (over 3.2-mm opening, over 2.8-mm opening, and through 2.8-mm opening, respectively).

Single-Kernel Characterization System

SKCS model 4100 isolates individual wheat kernels, weighs them, and crushes them in a progressively narrower gap formed by a toothed rotor and a crescent (Perten Instruments 1995). The

TABLE II
Cultivar, Class, Oven Moisture, Single-Kernel Characterization System (SKCS) Moisture, and SKCS Hardness Index for the 42-Sample Validation Set

Cultivar	Wheat Class[a]	Oven Moisture (%)	SKCS Moisture (%)	SKCS Hardness Index
Caldwell	SRW	13.2	12.7	6.7
Caldwell	SRW	13.2	12.4	7.6
Cardinal	SRW	11.7	11.7	8.5
Sawyer	SRW	11.7	11.7	9.3
Madison	SRW	11.8	11.8	9.5
Sawyer	SRW	13.1	12.6	9.7
Clark	SRW	11.7	11.4	12.4
Madison	SRW	13.1	12.7	12.4
Cardinal	SRW	12.9	12.5	16.4
P-2548	SRW	11.9	11.9	16.5
Clark	SRW	13.2	12.7	16.7
Sawyer	SRW	13.0	12.3	17.0
Cardinal	SRW	12.7	12.6	18.7
Clark	SRW	12.7	12.3	18.9
Madison	SRW	13.2	12.6	20.0
P-2548	SRW	13.3	12.6	21.3
Oasis	SRW	12.3	12.2	23.8
P-2548	SRW	13.1	12.4	26.7
Delta Queen	SRW	10.0	10.3	31.8
Compton	SRW	11.2	11.2	33.6
Nelson	SRW	10.8	10.9	34.2
Cardinal	SRW	10.4	10.0	36.2
Hart	SRW	11.4	11.3	40.4
Fillmore	SRW	10.9	10.9	42.3
Hillsdale	SRW	10.4	10.2	42.7
Scotty	SRW	11.4	11.4	44.4
Arthur	SRW	10.4	10.3	47.9
Beck 109	SRW	10.8	10.5	54.6
Hawk	HRW	10.2	10.3	51.0
Chisholm	HRW	10.5	10.5	54.6
HRW #210	HRW	10.1	10.1	59.1
Arkan	HRW	10.0	10.4	75.1
Wheaton	HRS	10.6	10.4	75.4
Marshall	HRS	10.5	10.5	76.0
Newton	HRW	9.9	10.0	76.3
T-Bird	HRW	9.9	10.2	76.7
Brandy	HRW	10.5	10.7	76.8
Vance	HRS	14.4	14.1	77.5
Butte 86	HRS	9.8	9.8	78.6
Guard	HRS	10.0	10.0	80.4
Stoa	HRS	10.0	10.2	83.6
Vic	Durum	11.7	11.6	89.9

[a] SRW = soft red winter, SWW = soft white winter, HRW = hard red winter, and HRS = hard red spring.

crushing force and electrical conductivity between the rotor and electrically isolated crescent are measured. Those data are processed by the integrated computer software for 300 kernels to provide the means and standard deviations for weight, size, moisture, hardness index, and hardness index distribution of all the kernels. The U.S. market classification is determined by the distribution of the individual kernel hardness measurements within four hardness ranges as suggested by the Federal Grain Inspection Service of the U.S. Department of Agriculture.

Each sample was submitted to the SKCS under normal operating parameters and conditions. Data were retrieved from the SKCS computer files that contained the recorded information of each kernel plus the means and standard deviations of each sample. A primary computer file contained the averages of the "raw data" for each sample and values for 12 measured parameters. They were designated as weight (mg), peak force (maximum load cell force, A/D count), conductivity (A/D count), area (area of the force-time crush profile, A/D count-second), GompA (Gompertz function coefficient A, a coefficient describing the intercept of the normalized cumulative frequency distribution of the first derivative value of the force-time crush profile, units), GompB (Gompertz function coefficient B, a coefficient describing the slope of the normalized cumulative frequency distribution of the first derivative value of the force-time crush profile, units), length (length of crush period, number of data points in the crush force profile), diameter (mm, diameter of kernel), moisture (%), hardness index (units), conductance (Smm, conductance × unit thickness), and crescent temperature (°F). Those values were used as variables for statistical analyses. All values were means of 300 kernels.

Statistical Analysis

Data were analyzed for descriptive statistics, analysis of variance, multiple linear regression, and simple linear correlation by the Winstar PC statistical software package (Anderson-Bell, Aurora, CO) and Statistica (StatSoft, Inc., Tulsa, OK). The regression equation was built using forward stepwise (P = 0.05) inclusion of parameters.

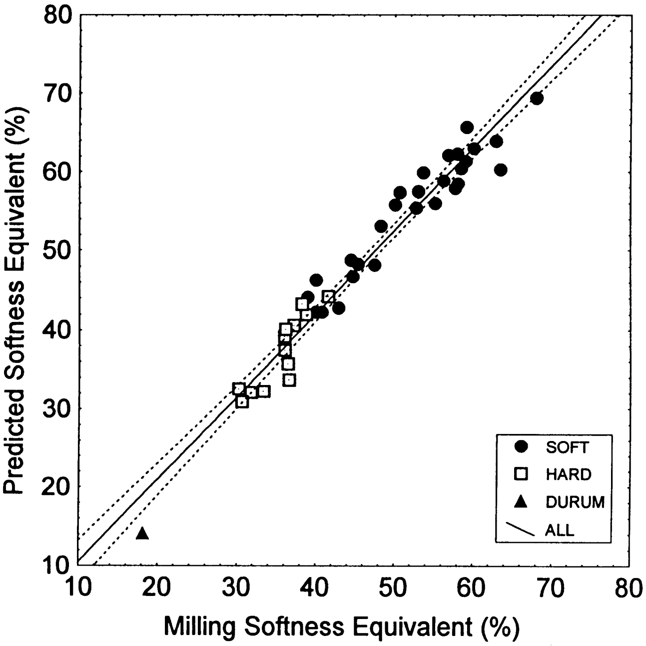

Fig. 1. Predicted and actual softness equivalent (SE) values for 28 soft, 13 hard, and one durum wheat. Greater SE values indicate softer grain texture. Dotted lines represent the 95% confidence interval of the regression.

RESULTS AND DISCUSSION

Equation Generation Set

A multiple linear regression equation was generated for predicting SE from the equation generation set of wheats. The parameters evaluated for inclusion were weight, peak force, conductivity, area, GompA, GompB, length, diameter, moisture, hardness index, conductance, and crescent temperature. Of those parameters, the following regression equation was generated using forward stepwise inclusion of parameters for predicting SE:

$$\begin{aligned}\text{Predicted SE} = 200.08 - 0.05874\ (\text{peak force})\\ - 155.08\ (\text{GompB}) + 0.000145\ (\text{area}) \quad (2)\end{aligned}$$

The equation had an r^2 of 0.982, a standard error of estimate of 2.12, and an F ratio of 236.5 ($P < 0.00001$). The mean and range for peak force were 1,013 and 1,898, respectively. The mean and range for GompB were 0.904 and 0.141, respectively. The mean and range for area were 277,955 and 569,835, respectively. Of the SKCS instrument parameters, these three terms best described the force-time crush profile. Other statistically significant and more complicated regression models were formulated that produced lower standard errors of prediction. Only the simplest three-term model was used in this report, because the three-term model produced no slope when residuals were compared against predicted values.

Verification Set

The predictive equation for SE was verified using a set of 42 wheats. The predicted values for SE versus actual milling SE values were highly correlated (r = 0.98, $P < 0.00001$) and the standard error of estimate was 2.58. Because the moisture content of a sample before milling shifts SE values higher for wetter samples and lower for dryer samples, milling SE values were adjusted to 14% moisture content. That allowed better correlation and comparison with milling data obtained from other systems of hardness evaluation and with larger millings systems for which wheat is tempered before milling. Without tempering or data adjustment to a common moisture content, estimates of wheat texture should not be compared with other data or methods. For example, the near-infrared spectroscopy standard method (AACC 1995) for evaluating wheat hardness must incorporate a moisture correction or tempering step (Windham et al 1991, 1993).

Thus, the predicted SE values also were subsequently regressed to a standard moisture value of 14%. The moisture values used for prediction values were obtained from SKCS data and the moisture values used for actual mill SE values were determined as oven moisture contents of the wheats before milling. The regression equation used for the moisture adjustment is as follows:

$$\text{Predicted adjusted SE (14\%)} = \text{SE} + [(14 - \text{moisture}) \times 1.08] \quad (3)$$

Figure 1 shows the predicted SE at 14% moisture versus the actual milling at 14% moisture. The correlation coefficient (r) was 0.98 ($P < 0.00001$) and standard error of estimate was 2.56. Analysis of residuals showed no bias versus predicted values for either hard or soft wheats.

Application of Predicted SE to Wheat Moisture Content

The predictive equation for SE was demonstrated on three sets of wheat samples that varied in wheat kernel texture. As mentioned in the introduction, several studies employing various approaches have shown that wheat kernels become softer as their moisture content increases. A set of four soft wheats was tempered to four to six moisture contents and analyzed using the SKCS. The SKCS hardness index values for those wheats indicated that, as moisture content increased, the two softer soft wheats (Excel and Ohio 490) became apparently harder (Fig. 2). Figure 3 shows the predicted SE values versus wheat moisture content for those wheats. As expected, as moisture content increased, the predicted SE values accurately indicated that the wheats became softer. Note that wheats with higher-moisture content could not be milled on the modified Quadrumat Jr.; thus the SE prediction was extended beyond the moisture range of the calibration sample set.

Application of Predicted SE to Wheat Kernel Size

As mentioned in the introduction, several studies employing various approaches have shown that smaller wheat kernels are often softer than larger kernels. Smaller kernels are usually softer for one or two primary reasons. One is shriveling. Shriveled kernels are smaller, have less endosperm content than plump nonshriveled kernels, and are softer.

Not all small kernels are shriveled. Another reason for softer, smaller kernels is the pressure for higher grain yield in modern cultivars. A common technique is to select for cultivars that produce a smaller tertiary row of kernels between two full-size rows. Those smaller kernels develop later than the kernels in the primary rows and are often softer because they have less time to produce full, plump kernels. Larger kernels develop toward the middle of the rachis in primary rows. They flower and develop first, mature faster, and tend to be harder than kernels at the top and bottom of the rachis, as well as those in tertiary rows (Gaines 1986).

Five subsamples of the soft wheat cultivar Pioneer 2510, nine subsamples of the soft wheat cultivar LB292, and five subsamples of the hard spring wheat cultivar Butte 86 were produced by sieving. The subsets of sized kernels were evaluated for TKW. The SKCS hardness index values for those subsets identified smaller kernels (lower TKW) as apparently harder (Fig. 4). However, smaller kernels had higher predicted SE values, accurately identifying them as softer (Fig. 5).

Three sets of Pioneer 2580 samples grown at three locations were sieved to produce subsets that had large, medium, and small kernels. Figure 6 shows that higher SKCS hardness index values suggested that smaller kernels were apparently harder. However, Figure 7 shows that small kernels had higher predicted SE values, accurately identifying them as softer than larger kernels.

The above evaluation of samples, varying in moisture content and kernel size, demonstrated the utility of a predictive SE equation (or other similar approach) for possible use as a basis for an SKCS wheat market characterization, especially among soft wheat samples that have high moisture content or have a relatively large proportion of small size kernels. Other direct measures of grain texture also may be predicted.

CONCLUSIONS

One of many excellent features of the SKCS model 4100 instrument is the large amount of "low level instrument data" that can be made accessible. This report demonstrated only one use of

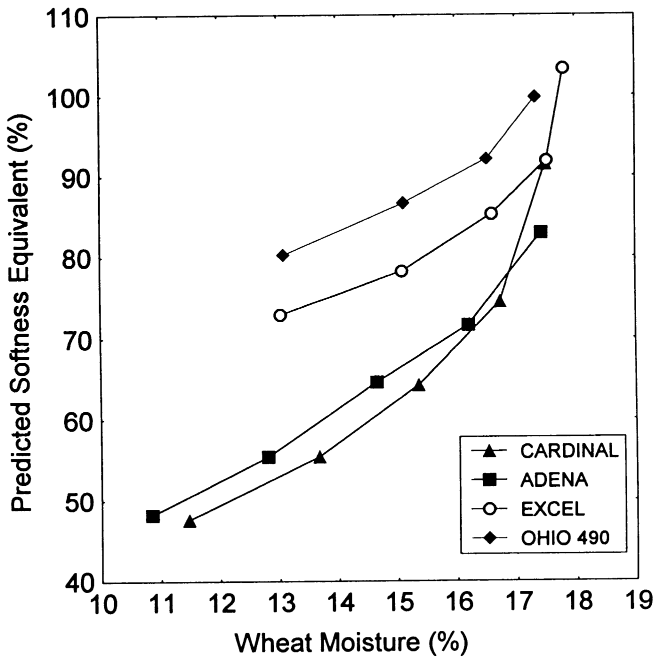

Fig. 3. Predicted softness equivalent (SE) values at several wheat moisture contents for four soft wheats. Greater SE values indicate softer grain texture. Predicted SE standard deviation = 0.75.

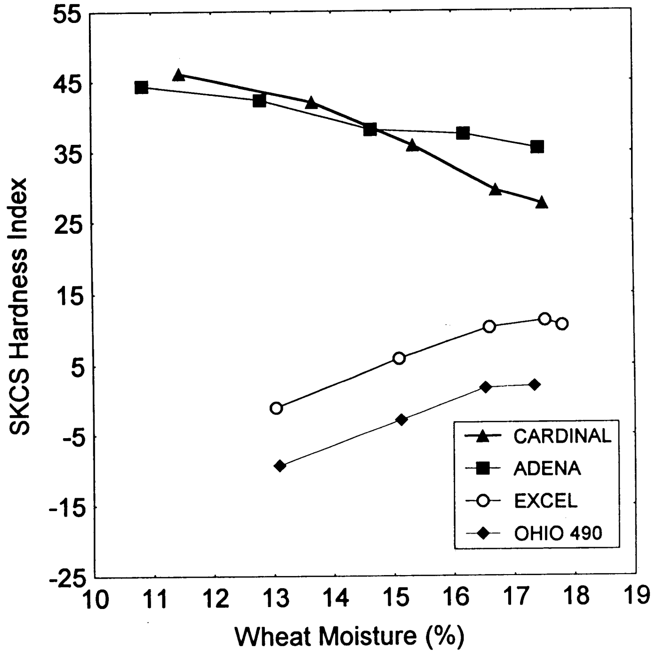

Fig. 2. Single-kernel characterization system (SKCS) hardness index values at several wheat moisture contents for four soft wheats. Smaller hardness index values indicate softer grain texture. Hardness index standard deviation = 1.51.

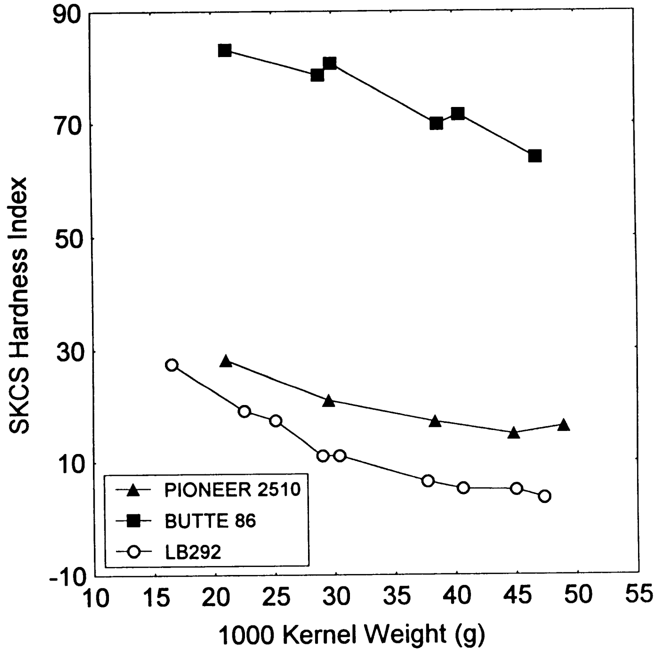

Fig. 4. Single-kernel characterization system (SKCS) hardness index values at several 1,000-kernel weights for two soft wheats (Pioneer 2510 and LB292) and a hard wheat (Butte 86). Smaller hardness index values indicate softer grain texture. Hardness index standard deviation = 1.28.

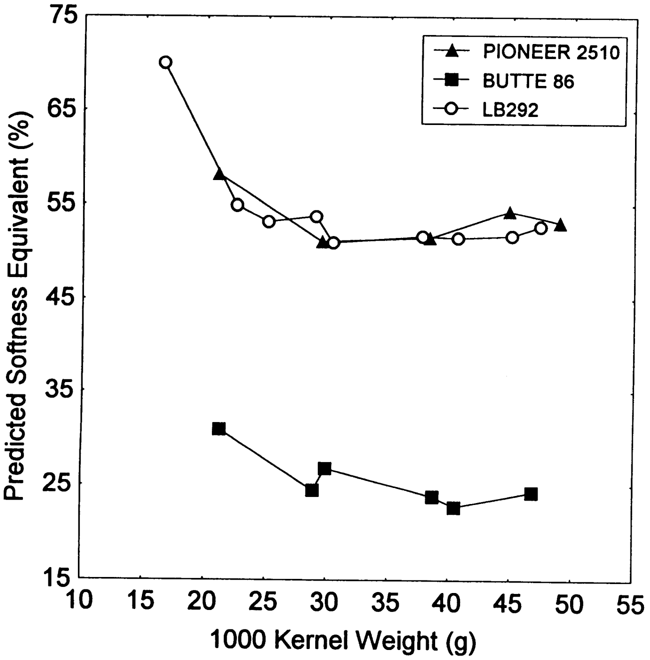

Fig. 5. Predicted softness equivalent (SE) values at several 1,000-kernel weights for two soft wheats (Pioneer 2510 and LB292) and a hard wheat (Butte 86). Greater SE values indicate softer grain texture. Predicted SE standard deviation = 0.96.

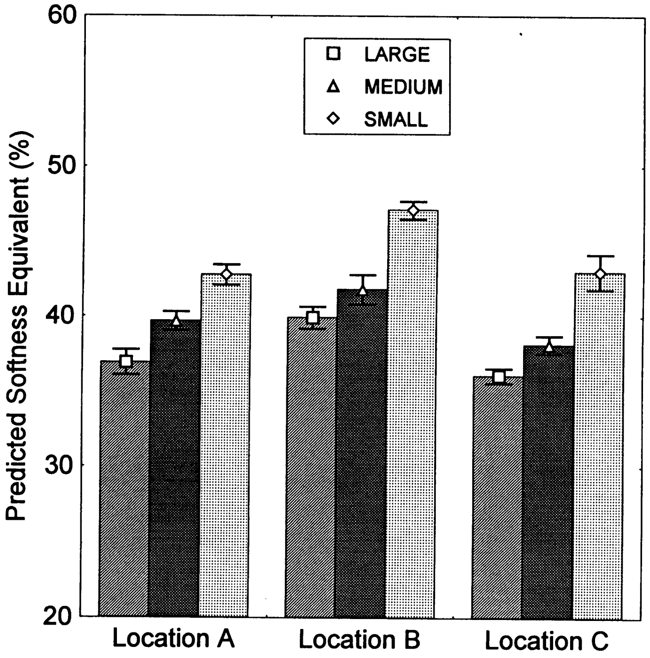

Fig. 7. Predicted softness equivalent (SE) values of large, medium, and small kernels for Pioneer 2580 grown at three locations. Greater SE values indicate softer grain texture. Error bars represent ± one standard deviation.

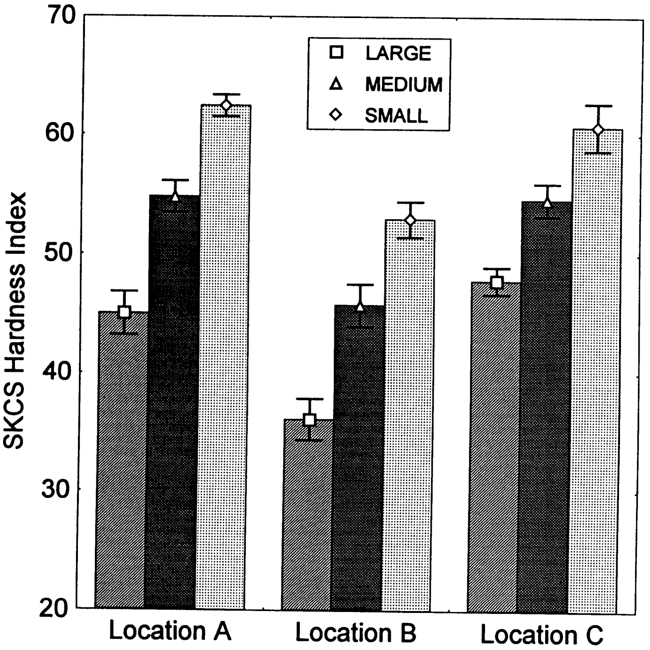

Fig. 6. Single-kernel characterization system (SKCS) hardness index values of large, medium, and small kernels for Pioneer 2580 grown at three locations. Smaller hardness index values indicate softer grain texture. Error bars represent ± one standard deviation.

some of those data (predicting an independent measure of kernel texture, i.e., SE derived from a modified Quadrumat Jr. mill and sieving system). Typically, the SKCS model 4100 classifies wheat grain samples into classes of hard, soft, or mixed wheat. Classification is based on a sophisticated algorithmic treatment of several parameters obtained during the crushing of individual kernels. Because of its design and construction, the SKCS model 4100 instrument generates a large amount of useful data from processing individual wheat kernels, as well as a useful mean and distribution information of bulk (300-kernel) samples. Portions of that information were found valuable in predicting the relative grain texture of the same samples analyzed by a different procedure, SE. The prediction equation was well validated on a larger set of wheat samples.

At this point, the SKCS instrument data appeared to be inaccurately influenced by kernel moisture content and kernel size when analyzing some soft wheats. Higher-moisture content may increase the hardness index values in a manner analogous to the increased work input observed when processing higher-moisture wheat through some grinding devices (Obuchowski and Bushuk 1980; Hook and Wallington 1981; Miller et al 1981a, 1982). Presently, new moisture calibration equations are being investigated. The prediction equation for SE does not use SKCS hardness index values and accurately reflects the influence of kernel moisture content and the size of soft wheat kernels. Other similar approaches could be attempted with SKCS data.

If the objective is to utilize the SKCS to produce a classification of wheat using the mean and distribution of force-deformation profile data from 300 kernels, the existing algorithms may prove generally satisfactory. However, especially for soft wheat, that approach could be augmented or replaced by a regression prediction of a different and independent texture measurement (i.e., SE). These findings support the expansion of the design, scope, and application of the SKCS 4100 instrument. The reported prediction equation also may be useful to predict actual milling grain hardness from very small samples (300 kernels).

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