

Application of the Single-Kernel Characterization System to Durum Wheat Testing and Quality Prediction

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ABSTRACT

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The Single Kernel Characterization System (SKCS 4100) measures single kernel weight, width, moisture content, and hardness in wheat grain with greater speed than existing methods and can be calibrated to predict flour starch damage and milling yield. The SKCS 4100 is potentially useful for testing applications in a durum improvement program. The mean SKCS 4100 kernel weight and moisture values from the analysis of 300 individual kernels gave good correlations with 1,000 kernel weight ($r^2 = 0.956$) and oven moisture ($r^2 = 0.987$), respectively. Although significant correlations were obtained between semolina mill yield and SKCS 4100 weight, diameter, and peak force, they were all very low and would be of little use for prediction purposes. Similarly,

although there were significant correlations between some SKCS 4100 parameters and test weight and farinograph parameters, they too were small. The SKCS 4100 has been calibrated using either the single kernel hardness index or crush force profile to objectively measure the percentage vitreous grains in a sample with reasonable accuracy, and it correlates well with visual determination. The speed and accuracy of the test would be of interest to grain traders. An imprecise but potentially useful calibration was obtained for the prediction of semolina mill yield using the SKCS 4100 measurements on durum wheat. The SKCS 4100 is useful for some traits such as hardness, grain size and moisture for early-generation (F3) selection in a durum improvement program.

The evaluation of durum (*Triticum turgidum* L., ssp. *durum* Desf.) breeding lines for quality in the Australian National Durum Wheat Improvement Program, Tamworth, NSW, involves a series of tests of varying complexity and expense. It would be desirable to develop more rapid and economical methods to predict end-use quality. In the program at Tamworth, grain size was measured as 1,000 kernel weight grain hardness using a pearlograph (Chesterfield 1971, Pearson and Wedd 1978), and grain protein and moisture content was measured by near-infrared reflectance spectroscopy (NIR). These tests give an estimate of the whole sample but do not measure individual kernels and thus do not provide any information on sample uniformity. Selection for those crossbreeds that give a small range in grain size distribution, for example, should produce a more uniform grain size, which millers claim to be more acceptable as such lots of wheat condition more evenly and mill more efficiently.

The Single Kernel Characterization System (SKCS) 4100 (Perten Instruments North America Inc., Springfield, IL) was developed for the measurement of single kernel weight, width (either lateral or longitudinal depending on the orientation of the kernel when it reaches the crescent), moisture, and hardness in wheat (Martin et al 1993). This technology provides the possibility of obtaining data on the uniformity of a grain sample with essentially the same speed as bulk tests that offer an average value only. The SKCS 4100 is a potentially useful tool to a plant breeder by maximizing the number of tests conducted simultaneously and providing useful mean and distribution information on bulk (300 kernel) samples. The SKCS 4100 can be used to measure single kernel hardness index (SK-HI), single kernel moisture content (SK-MC), single kernel weight (SK-WT), and single kernel diameter (SK-DM). In the SKCS analysis, a small sample (≈ 20 g) of grain is deposited into a hopper where a rotating wheel (with the aid of a vacuum) picks up individual kernels and deposits them one at a time into a weighing boat. After weighing, the kernel passes down an inclined crescent where the diameter is measured and the kernel is then crushed between the crescent and a toothed rotor. A load cell measures and records the crush force-time profile. A

sample comprising a preset number of kernels (usually 300) are individually analyzed in 3-5 min and the data presented as a distribution with mean and standard deviation calculated for each of the four measurements. Results of recent work have indicated that calibration equations may be derived to predict wheat texture (Gaines et al 1996), flour milling yield (Satumbaga et al 1995, Osborne et al 1997), and starch damage (Osborne et al 1997) from the SKCS 4100 data.

In durum wheat, the proportion of vitreous durum kernels is an important parameter for high semolina milling yield and maintaining quality of the derived pasta. Vitreous durum kernels appear glassy and translucent due to the compact structure of the protein matrix and starch granules. Nonvitreous or starchy kernels are opaque due to air spaces between starch granules (Dexter et al 1989). When milled, starchy kernels reduce to fines, decreasing semolina extraction (Dexter and Matsuo 1981). The estimation of vitreous kernel content in durum wheat is an important international grading factor and is performed by visual inspection (ICC 1995), which is a subjective and tedious procedure. Since the SKCS 4100 provides data related to kernel hardness, it should be possible to develop a calibration to measure durum vitreousness, a more rapid and objective method than visual assessment.

The aim of this work was to evaluate the utility of the SKCS 4100 in a durum breeding program and, specifically, to develop new calibrations to predict kernel vitreousness and semolina mill yield.

MATERIALS AND METHODS

Samples

Several sample sets were used in this study. Each set was selected to enable different issues to be addressed.

Set 1 (repeatability) assessed the repeatability of each SKCS parameter. Six durum crossbred lines grown at two different sites were analyzed repeatedly ($n = 20$) by one operator.

Set 2 (accuracy) assessed the accuracy of the SKCS weight. A subset of 50 samples from Set 5 was used for which 1,000 kernel weight data were available. In addition, the distribution in kernel weight was obtained from a 300-kernel sample where the weight of each kernel was measured on an analytical balance and the SK-WT was obtained by the SKCS 4100. The SK-DM measurement of 300 individual kernels was compared with manually measured diameter of each kernel using digital calipers. To assess the accuracy of the SKCS 4100 moisture content measurement a sample set of 36 samples was prepared. Each durum wheat sample was cleaned using a Carter-Day dockage tester (Simon Carter Co.,

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Minneapolis, MN). Grain <6 mm (No. 25 screen) and >2 mm was divided into aliquots of 100 g. Samples were either partly dried in an oven at 50°C or had water added (1–6% by weight) to achieve final moisture percentages of 8–16%. The sample (100 g) was sealed in a plastic screw-capped container (11 x 4 cm) and mixed by hand by inverting continuously for 5 min to disperse the water evenly over the surface of the grain. Four hours later, the container was again mixed for 5 min. The tempered wheat was stored overnight at room temperature. The moisture content of a subsample was determined by oven-drying (Approved Method 44-15A, AACC 1995); the SK-MC was obtained concurrently on the equilibrated samples. For comparing pearlograph hardness to SKCS hardness, all 584 lines from Set 4 were evaluated.

Set 3 (vitreousness) was used to develop a durum vitreousness calibration. Two subsets were prepared (one in each of the collaborating laboratories).

In the first subset, a commercial sample of durum was first separated into 100% vitreous and 100% nonvitreous fractions by visual identification of individual kernels. From each of these two fractions, a calibration set was prepared by mixing vitreous with nonvitreous grains to form a 300-kernel samples of 0, 25, 50, 75, 85, 90, 95, 98, and 100% vitreousness. Each 300-kernel sample was analyzed using the SKCS 4100, and the mean SK-HI was calculated. The determination of %vitreousness by visual inspection was a modification of a method produced by AWB Ltd. (Melbourne, Australia). A 300-kernel sample was obtained and separated into vitreous, mottled, and bleached fractions. Occasionally, kernels from the bleached fraction were split lengthwise by a scalpel, and any kernel with opaque starchy areas inside was classed as mottled. Grain was screened through a 2.0-mm slotted screen, and 300 kernels were counted and classified as vitreous or nonvitreous. Vitreous kernels are bright and translucent with a uniform amber color. Starchy or nonvitreous kernels have opaque areas with a dull yellow appearance. Bleached kernels are dull with a pale washed-out appearance. To distinguish starchy from bleached kernels, it was sometimes necessary to cut the bleached kernels longitudinally; those with any opaque areas were classed as starchy. The %vitreousness was defined as the proportion of vitreous kernels in a 300-kernel sample. Another set of samples was obtained to test the SKCS vitreous calibration (prediction set) consisting of 22 samples of commercial durum (supplied by GrainCorp Operations Ltd., Narrabri, NSW) where %vitreous count was determined visually.

For the second subset, three samples of Australian durum were obtained from three different farms in New South Wales. A further five samples were obtained from the Cereals Institute, Greece, in the course of a ring test on ICC Standard No. 129 (ICC 1995). These eight samples were analyzed (five replicates) for %vitreousness by ICC Standard No. 129. Two of the Australian samples and four of the ICC samples were separated into 100% vitreous and 100% nonvitreous fractions by visual identification of individual kernels. Nineteen mixtures of varying %vitreousness (0, 25, 50,

75, 85, 90, 95, 98, and 100%) were then prepared by counting the appropriate proportions of kernels to form a 200-kernel sample for analysis by the SKCS 4100 to produce a set of 27 samples in total.

Set 4 was constructed to relate farinograph data (Approved Method 54-21), grain protein, and hL weight to SKCS parameters. Of the 584 lines from set 5, only 280 samples were available to relate these properties to SKCS parameters. In this set of 280 samples, there were 32 tetraploid accessions (Sissons et al 1998).

Set 5 (breeding material) was a calibration sample set used to determine whether the SKCS 4100 could be used to predict semolina mill yield (SY%). This set was made up of 584 crossbreeds at an advanced (F5 to F7) stage of breeding over several years (1993–1997) and 32 genetically diverse tetraploid wheats (Sissons et al 1998). After cleaning on a Carter-Day dockage tester (settings as for Set 2), tests included 1,000 grain weight (weight of 250 kernels × 4), pearlograph grain hardness (Chung et al 1975, Kuhlman et al 1979), grain protein by NIR (Approved Method 39-10), and hL weight. Grain was milled into semolina using a laboratory mill (Buhler MLU 202) (Approved Method 26-41). SY% was expressed on a total products basis.

SKCS 4100 Measurements

SKCS 4100 measurements were carried out according to the operating manual (Perten Instruments 1995), using 300 grains. Types of data recorded were: 1) four default measurements (SK-HI, SK-MC, SK-WT, SK-DM); 2) raw data used to calculate the default measurements (X-array); 3) X-array expanded to 40 variables with the use of transform functions such as exponentials, logarithms, inverse terms and ratios (Big File).

Sample Sets 1 and 2 were used to assess the precision and accuracy of the default measurements and Set 4 was used to derive simple correlations between the default measurements and grain and semolina quality characteristics.

Sample Sets 3 and 5 were used to develop new calibrations for vitreousness and semolina yield. The latest version of the instrument software (5.00C) allowed user calibrations to be installed but could only accept equations derived directly from the X-Array data using multiple linear regression. Therefore, a computer file was collected containing the averages of the X-array variables weight (mg), peak force (maximum load cell force, A/D counts), conductivity (A/D counts), area (area of the crush force profile, A/D count-second), GompA (Gompertz function coefficient A, a function describing the intercept of the normalized cumulative frequency distribution of the first derivative value of the crush force-time profile), 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), length (length of the crush period, number of data points in the crush force profile), diameter (mm), (equivalent to the breadth of the kernel), crescent temperature (°F), and DyFraction (time interval that a kernel exerts force on the crescent). Because the

TABLE I
Precision of Single-Kernel Characterization System (SKCS) Parameters for Durum Grain^{a,b}

Sample	SK-WT (mg)		SK-DM (mm)		SK-HI		SK-MC (%)	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
1	45.5	0.89	2.98	0.034	87.2	1.03	10.6	0.03
2	38.1	0.87	2.68	0.036	88.2	1.07	9.5	0.09
3	51.1	0.79	3.01	0.037	86.9	0.82	10.5	0.04
4	41.7	1.10	2.76	0.041	92.5	0.91	9.5	0.03
5	37.9	0.65	2.66	0.030	91.1	0.95	9.5	0.04
6	48.8	0.85	3.05	0.033	90.7	0.95	10.2	0.02
Overall mean	43.8		2.87		89.4		10.0	
Pooled SD	0.85		0.034		0.95		0.041	
CV% (range) ^c	1.54–2.64		1.10–1.54		0.95–1.22		0.22–0.95	

^a Six different samples of durum wheat were each analyzed 20 times. Mean and standard deviation (SD) of the *n* = 20 samples were calculated.

^b SK-WT = single kernel weight; SK-DM = single kernel diameter; SK-HI = single kernel hardness index; SK-MC = single kernel moisture content.

^c Coefficient of variation.

acquisition of the crush force A/D count versus time data is too slow relative to the speed of the singulator, only summary data (peak force, peak area, GompA, and GompB) are stored in routine use. These summary data together with average kernel weight were used in multiple regression analysis to predict %vitreousness and SY%

Statistical Analysis

The X-array data were imported into Excel v7 (Microsoft Corporation, Redmond, WA) and the resulting Excel spreadsheets were imported into Minitab v. 11 (Minitab Inc., State College, PA). Simple correlations and multiple linear regression equations were calculated using the method of least squares. Where selection of terms to be included in the regression equation was indicated, this was calculated as the residual sums of squares for all possible regressions with one or more terms. Then, using the residual sum of squares to compare equations with the same number of terms, the best one-term, two-terms, etc., equations were identified.

RESULTS AND DISCUSSION

Precision and Accuracy of SKCS 4100 Measurements

The mean and standard deviation (SD) for each of the six durum samples of Set 1 after repeated analysis ($n = 20$) and the pooled SD of repeatability for kernel weight (SK-WT), diameter (SK-DM), hardness (SK-HI), and moisture (SK-MC) are given in Table I.

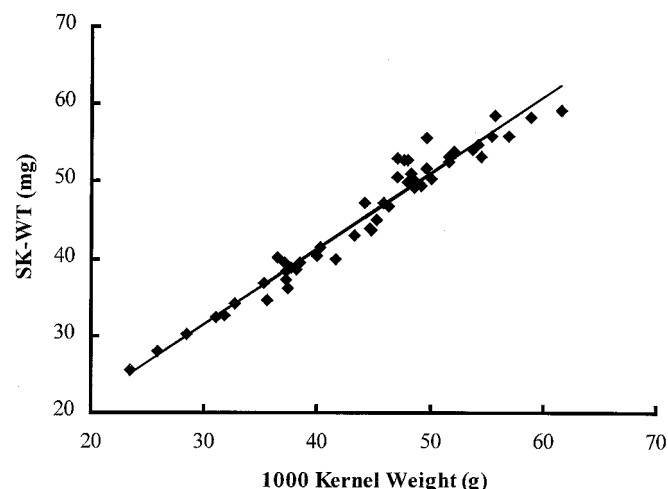


Fig. 1. Linear regression plot of single-kernel characterization system (SKCS) single kernel weight (SK-WT) vs. 1,000 kernel weight. SK-WT = $2.18 + 0.978 \times 1,000$ kernel weight; $r^2 = 0.956$, $n = 50$, relative standard deviation = 1.83 g.

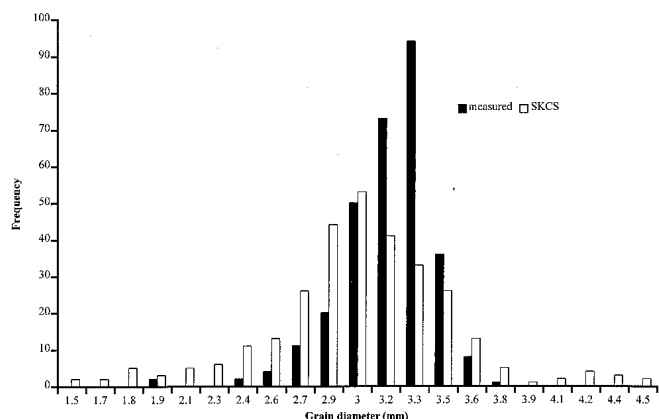


Fig. 2. Frequency distribution of the diameter of individual durum kernels in a sample measured using the single-kernel characterization system (SKCS) single kernel diameter (SK-DM) and measured with calipers.

When expressed as the coefficient of variation (CV%), the repeatability of all the SKCS parameters is very low (CV% = 0.2–2.7%), indicating excellent precision. The precision reported for durum is similar to that obtained for bread wheat (Osborne et al 1997).

The SKCS 4100 is factory-calibrated for common wheat. Therefore, it is necessary to verify the accuracy of these calibrations for each different grain type and to make skew or bias adjustments if required. Accuracy was determined by comparing the SKCS measured data with standard physical testing methods used in the Tamworth laboratory from sample Sets 2 and a subset of Set 4.

The SKCS weigher operates on the principle that a kernel dropped into the plastic weighing boat causes the boat to depress, and the electrical force required to return the boat to a horizontal position is proportional to the mass of the kernel. Therefore, SK-WT is a secondary measurement that requires calibration against an analytical balance. The distribution in kernel weight obtained from two 300-kernel samples measured using an analytical balance and the SKCS SK-WT data were compared. Both samples produced virtually identical comparisons (data not shown). There was an excellent agreement between the two methods with no significant difference ($P < 0.05$) in the means determined by unpaired t -test and a small residual standard deviation of the differences. There was an excellent correlation ($r^2 = 0.956$) and low residual standard deviation (RSD) of 1.83 g between SK-WT and 1,000 kernel weight (Fig. 1) for durum similar to that reported for bread wheat (Osborne et al 1997). The equation was SK-WT = $2.18 + 0.978 \times 1,000$ kernel weight, where the slope and bias are not significantly different from a slope of 1.0 and a bias of 0.0 at $P < 0.05$.

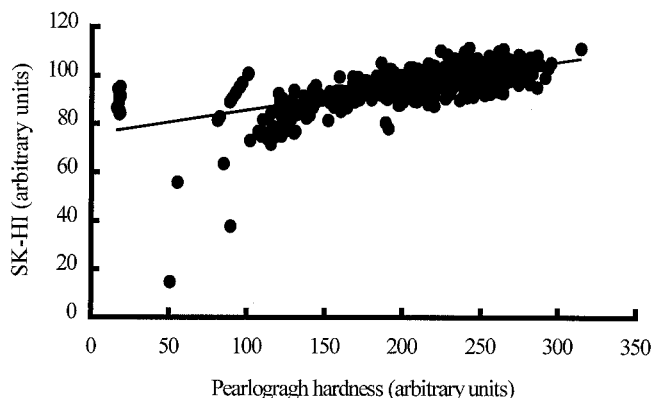


Fig. 3. Linear regression plot of single-kernel characterization system (SKCS) measured SK-HI vs. Pearlograph hardness. $r^2 = 0.462$, $n = 584$, relative standard deviation = 5.97.

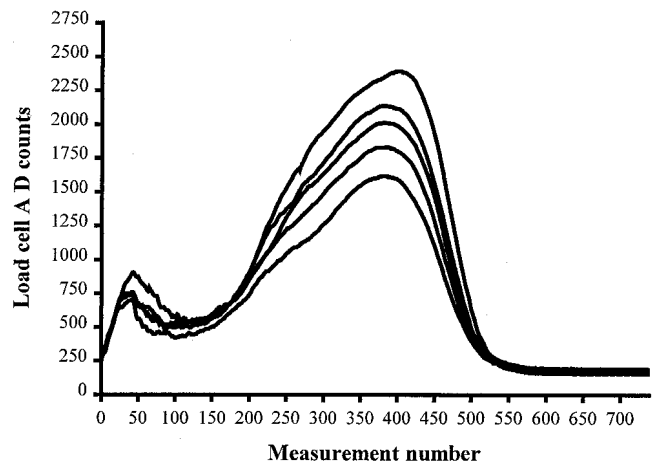


Fig. 4. Crush force profiles for samples of Australian durum (AD) with different %vitreousness. Each trace is the average of 200 kernels. Trace furthest from x-axis at measurement number 350 is the 100% vitreous sample, followed in order moving closer to the x-axis by 68, 40, 30, and 0%.

The diameter measurement of the kernel is based on the width at the point of first contact in the gap formed between the crescent and the rotor arc. This point is determined by the number of data scan intervals from contact to exit. A distribution of SK-DM obtained from the analysis of ≈300 kernels was compared to manually measuring the diameter of the same 300 kernels using digital calipers (Fig. 2). The SKCS 4100 assigned a number of kernels to sizes >3.5 mm and <1.8 mm, whereas no kernels were >3.8 and <1.8 mm when measured with calipers. Some error would arise in the manual measurement because kernels vary in shape, and it would not always be possible to obtain an accurate measure of diameter. On the other hand, the SKCS diameter measurement will be influenced by the orientation of the kernel as it enters the crescent. An unpaired *t*-test revealed a difference in the means ($P < 0.05$) of the two methods of measurement reflecting the above differences.

The SK-MC measure is accurate ($r^2 = 0.987$; RSD = 0.18%) over a broad range of moisture values. The equation was SK-MC = $1.045 \times \text{oven moisture} - 0.06$, where the slope and bias are not significantly different from a slope of 1.0 and a bias of 0.0 at $P < 0.05$.

The SK-HI measure is based on the crescent load cell A/D counts measured over a period of 125 msec. The raw data can be

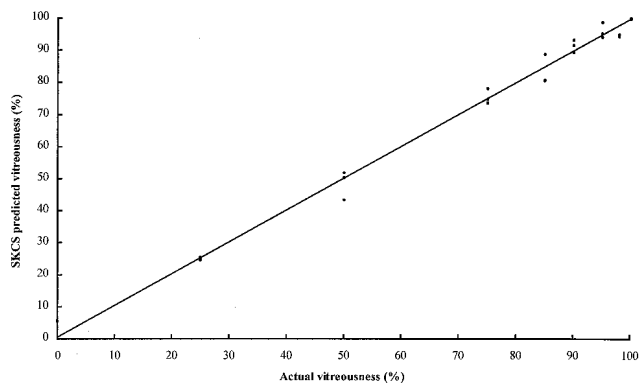


Fig. 5. Linear regression between average weight and average Gompertz B of 27 different mixtures of durum grain. %Vitreousness = $-3841 - 2.6 \text{ Avgwt} + 4262 \text{ AvggB}$; $r^2 = 0.993$, $n = 27$, relative standard deviation = 2.953.

recorded and plotted as a force-time crush profile. The peak force and the area under the curve is a measure of the energy required to crush the kernel; the harder the kernel the greater this energy. The selection of a numeric scale for SK-HI is used for the purposes of classification of wheat kernels into soft and hard and was based on the earlier use of an arbitrary scale for wheat hardness by NIR (Approved Method 39-70A). The Tamworth laboratory has been using a pearlograph to measure grain hardness but this does not give a strong correlation ($r^2 = 0.46$) with SK-HI (Fig. 3). The graph shows some clusters of anomalous data for which the most likely explanation is that the two methods measure different aspects of grain hardness (i.e., the pearlograph measures the kernel's resistance to abrasion, whereas the SKCS 4100 measures the force deformation profile during the crushing of the kernel). Furthermore, the SKCS 4100 was optimized to detect mixed hard and soft common wheat; durum was not included in the original

TABLE III
Mean ($n = 280$), Standard Deviation (SD), and Range of Single-Kernel Characterization System (SKCS), Milling, and Dough Rheology Characteristics of Durum Wheat Samples^{a,b}

Characteristic	Mean	SD ^c	Minimum	Maximum
Peak force	1,907.0	271.0	760.0	2,921.0
SK-WT (mg)	38.2 (10.8)	5.7	25.5 (7.6)	59.2 (16.3)
SK-DM (mm)	2.6 (0.5)	0.2	2.1 (0.4)	3.4 (0.7)
SK-HI	96.2 (15.1)	8.2	14.6 (0.5)	111.2 (18.9)
SK-MC (%)	11.4 (0.3)	0.4	10.1 (0.2)	13.1(0.4)
HW (kg/hL)	79.1	1.9	72.3	83.9
Grain protein (%)	14.4	1.2	10.6	18.2
DDT (min)	3.4	0.7	1.2	5.0
B ₁₀ (BU)	57.4	29.6	20.0	180.0
FWA (%)	60.6	2.2	55.3	67.8
Total mill yield (%)	79.7	2.0	64.7	86.6
SY%	68.2	2.7	43.3	75.6

^a SK-WT = single kernel weight; SK-DM = single kernel diameter; SK-HI = single kernel hardness index; SK-MC = single kernel moisture content. HW = hectoliter weight; DDT = Farinograph dough development time; B₁₀ = break-down after 10 min; FWA = farinograph water absorption; SY% = semolina mill yield percentage.

^b For each of the 280 samples analyzed, the SKCS gave a mean and standard deviation from the analysis of 300 kernels. The average of these 280 standard deviation values is shown in parentheses.

^c Standard deviation calculated for the data from the 280 samples.

TABLE II
Visual vs. Single-Kernel Characterization System (SKCS) Methods to Measure Durum Vitreousness^a

Sample No.	Visual (%)	SKCS		Classification into Grade ^b		
		M1 (%)	M2 (%)	Visual	M1	M2
13	60	92	78	Unclassified	ADR1	ADR3
20	66	69	74	Unclassified	ADR3	ADR3
3	75	74	92	ADR3	ADR3	ADR1
21	76	81	89	ADR3	ADR2	ADR2
9	77	76	98	ADR3	ADR3	ADR1
15	84	100	87	ADR2	ADR1	ADR2
22	84	93	97	ADR2	ADR1	ADR1
2	86	97	100	ADR2	ADR1	ADR1
6	89	99	88	ADR2	ADR1	ADR2
8	89	88	100	ADR2	ADR2	ADR1
11	89	89	100	ADR2	ADR2	ADR1
17	90	98	92	ADR1	ADR1	ADR1
18	90	92	99	ADR1	ADR1	ADR1
1	92	95	100	ADR1	ADR1	ADR1
19	92	100	90	ADR1	ADR1	ADR1
5	93	91	100	ADR1	ADR1	ADR1
14	94	94	98	ADR1	ADR1	ADR1
4	95	94	100	ADR1	ADR1	ADR1
12	97	92	94	ADR1	ADR1	ADR1
7	98	92	100	ADR1	ADR1	ADR1
10	98	96	100	ADR1	ADR1	ADR1
16	98	90	93	ADR1	ADR1	ADR1

^a Predicted % vitreous kernels using SKCS hardness index calibration equation M1 or X-ray data equation M2.

^b Classification based on Australian durum grading system ADR1 ≥ 90%; ADR2 80–89%; ADR3 75–79%; no classification <75%.

calibration. A Tamworth-specific method was used in this study due to the lack of a fundamental reference method. However, a more suitable physical test for accuracy comparison would be PSI because a good correlation was found between PSI and SK-HI in bread wheats (Osborne et al 1997, Williams et al 1998).

In summary, the SKCS 4100 provides accurate and reliable data on durum grain, weight, and moisture from as little as 300 grains and can be used to replace the more time-consuming methods previously used in a durum quality testing laboratory. Its implementation would reduce the time required for analysis. It is not possible to comment on the accuracy of the SKCS 4100 for diameter and hardness due to lack of fundamental reference methods.

Prediction of Durum Vitreousness Using the SKCS 4100

Vitreousness in durum is an important international grading factor and a high percentage of vitreous kernels (>90%) is desired. The system used in Australia has three grades: ADR1 (Australian Durum Grade 1) $\geq 90\%$, ADR2 80–89%, ADR3 <79% (AWB Ltd., Australia). Starchy durum tends to be lower in protein content than vitreous durum wheat (Dexter et al 1988), imparting poor cooking quality to pasta (Matsuo and Dexter 1980, Dexter and Matsuo 1981). Several studies have shown that starchy durum wheat is softer than vitreous durum wheat (Matsuo and Dexter 1980, Dexter and Matsuo 1981, Dexter et al 1988), so rapid methods to measure grain hardness would be a useful alternative to the visual assessment of vitreous kernels.

Using sample Set 3 (subset 1), vitreousness was measured at 0, 25, 50, 75, 85, 90, 95, 98, and 100%, with hardness varying from 95–52 SK-HI index units. Of particular interest is whether the SKCS 4100 can discriminate samples within the range of vitreousness of the commercially useful range of 75–90% to classify grain lots into one of the three grades. The calibration set gave an excellent correlation was obtained ($r^2 = 0.993$) (Eq. M1: %Vitreousness = $0.395 \text{ SK-HI} + 54.667$) between SK-HI and %vitreous durum kernels.

Using sample Set 3 (subset 2), crush force profiles plotted as load cell A/D counts versus measurement number (Fig. 4) confirmed that a greater force is required to crush the vitreous kernels than with the nonvitreous kernels. There was also a systematic relationship between %vitreous kernels in a sample and the shape of the crush force profile. X-Array data were used to construct a multiple regression equation to predict vitreousness. Examination

of all possible combinations of terms produced a two-term equation (Eq. M2, Fig. 5): $\% = -3841 - 2.6 \text{ AvgWt} + 4262 \text{ AvggB}$, $r^2 = 0.993$, $\text{RSD} = 2.953$, $P < 0.001$, where AvgWt is average grain weight; AvggB is average Gompertz function coefficient B performed as well as the equation containing all five X-array terms describing the kernel weight and crush force profile. Weight is required in the prediction to correct for the fact that larger kernels require a greater force to crush them, but only one of the functions that describe the force crush profile was required as these were all very highly intercorrelated ($r > 0.97$).

To evaluate both equations M1 and M2, a prediction set of 22 samples of commercial durum (Set 3) with starchy kernels present was assessed visually for %vitreous kernels and analyzed by the SKCS 4100. This sample set exhibited a visual percentage vitreousness count of 60–98% (Table II). Using %vitreous kernel ranges applicable to marketing (samples 13 and 20 were excluded), the two SKCS calibrations were compared with the visual method. There was a 25% error rate of prediction using equation M1 and a 35% error rate for M2. Equation M1 gave a lower error than M2 in this limited sample set and would be a better choice as a calibration method. A possible explanation for these discrepancies is that with the visual method, kernels are classified as starchy even when a small portion of the kernel is affected. However, to the SKCS 4100, this type of kernels has hardness similar to vitreous kernels and therefore the SKCS 4100 would give a higher %vitreousness estimation. From a breeder's viewpoint, this is preferable to rejecting vitreous lines, but not from a marketer's perspective. It should be noted that the classification system between the three grades is rigid in that a vitreousness of 89 vs. 90% gives a different grading. Whether there is any difference in quality between a value of 90 vs. 89% is not known, but it would seem unlikely. It would be more reasonable to have a range of overlap. The preliminary results show that the SKCS 4100 could be used to measure %vitreousness in a sample of durum, but the calibration needs to be further assessed with a larger prediction set. The SKCS 4100 would be a more reliable and objective method compared to the visual approach.

Relationships Among Single Kernel Characteristics with Wheat and Semolina Parameters

Advanced durum breeding lines and a diverse set of tetraploid accessions (Set 4) ($n = 280$ samples) were evaluated for hL weight (HLW), grain protein (NIR), total mill yield, and SY%, Farinograph dough development time (DDT), breakdown after 10 min (B_{10}), water absorption (FWA), and the five SKCS mean

TABLE IV
Simple Correlation Coefficients Among Single-Kernel Characterization System (SKCS) Measurements ($n = 280$)^a

	Peak Force	SK-WT	SK-DM
SK-WT (mg)	0.88** ^b	1.00	
SK-DM (mm)	0.84**	0.96**	1.00
SK-HI	0.18**	-0.24**	-0.19**

^a SK-WT = single kernel weight; SK-DM = single kernel diameter.

^b * and ** = Correlation coefficients significant at $P < 0.05$ and 0.01 , respectively.

TABLE V
Linear Correlation Coefficients ($n = 280$) Between Standard Quality Tests and Single Kernel Parameters^a

Characteristic	Single Kernel Parameters		
	Peak Force	SK-WT (mg)	SK-DM (mm)
HW (kg/hL)	ns ^b	0.20**	0.27**
SY%	0.54**	0.37**	0.36**
DDT (min)	-0.28**	-0.31**	-0.26**
B_{10} (BU)	0.35**	0.38**	0.34**
FWA (%)	0.50**	0.43**	0.38**

^a HW = hectoliter weight; SK-WT = single kernel weight; SK-DM = single kernel diameter; DDT = farinograph dough development time; B_{10} = breakdown after 10 min; FWA = farinograph water absorption, 11% moisture basis; SY% = semolina mill yield percentage.

^b ** = significant at $P < 0.01$; ns = not significant.

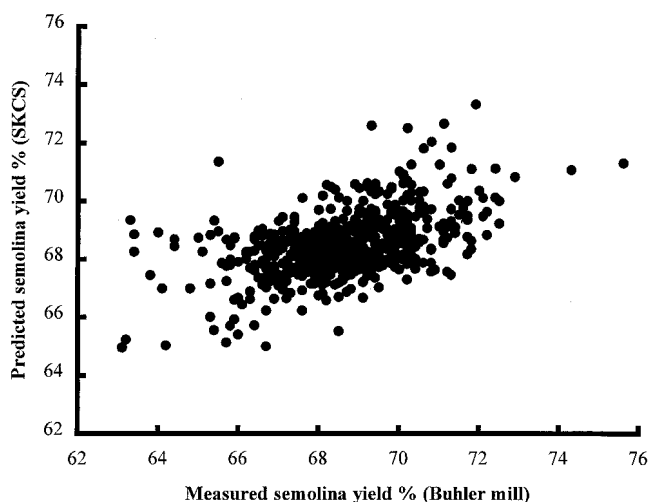


Fig. 6. Plot of fitted semolina mill yield predicted from analysis of single-kernel characterization system (SKCS) low-level machine data vs. semolina mill yield % measured by a laboratory mill.

parameters (SK-PF, SK-WT, SK-DM, SK-HI, and SK-MC). The means and ranges of these physical and chemical characteristics are summarized in Table III. It should be noted that the very low hardness values found for some samples were from species other than *T. turgidum*. The presence of the 32 diverse tetraploid species in the 280 samples extended the range in all parameters measured over that obtained from the breeding population. The SD values of SKCS parameters were calculated by the instrument software for each sample, and this gave an indication of the variation in the sample. Simple linear correlation coefficients among the SKCS parameters (Table IV) show that peak force had a significant positive correlation with SK-WT ($r^2 = 0.77$), SK-DM ($r^2 = 0.71$), because larger kernels require a greater force to crush, but a low correlation with SK-HI ($r^2 = 0.03$). The weight and size of the kernels were highly correlated, as would be expected. SK-HI was only weakly negatively correlated with SK-WT and SK-DM, and although the correlations were significant, grain size or weight explains very little of the variation in grain hardness. The correlations were improved by removing data for the tetraploid set (SK-HI vs. SK-WT, $r^2 = 0.20$ and SK-HI vs. SK-DM, $r^2 = 0.19$) but they were still very low. In hexaploid wheats, smaller kernels have been reported to be softer (Gaines et al 1996).

The simple linear correlation coefficients among wheat and semolina properties are shown in Table V. Although HLW was correlated with grain weight (SK-WT) and diameter (SK-DM), the r^2 values were very small. These results are in contrast to a study relating SKCS parameters to hard winter wheats (Ohm et al 1998). Also in a recent report (Troccoli and di Fonzo 1999), the test weight of 16 durum cultivars was not correlated with the mean individual kernel weights and kernel width.

Grain protein was not correlated with any of the SKCS parameters, and SK-HI was only weakly correlated with SY%. Significant correlations were obtained between peak force, SK-WT and SK-DM, and the three farinograph parameters, but again the r^2 values were only 0.25–0.07. Semolina mill yield was positively correlated with peak force, SK-WT, SK-DM, and SK-HI. Peak force gave the highest correlation coefficient with SY% but still explains <30% of the variation in SY%. A similar observation was found in a study of 12 hard winter wheats grown at six locations in Kansas (Ohm et al 1998). Employing a multiple linear regression model to predict SY% from peak force, SK-WT, SK-DM, and SK-HI, a significant but low correlation ($r^2 = 0.08$) was obtained that would not have practical use in predicting SY%. The results show that the SKCS durum parameters are related to conventional quality characteristics, but because of the low r^2 values, they would not be adequate for prediction purposes. Selection for a smaller range (lower SD) or uniformity for grain size, weight, and hardness could be useful when breeding for grain with more uniformity. This may improve the consistency of quality across different growing environments.

Prediction of Semolina Milling Yield

There is potential to develop a calibration for predicting SY% using the SKCS because a calibration to predict flour yield has already been reported (Osborne et al 1997). A calibration set (Set 5) of 584 durum breeding lines, for which SY% data were available, was used. The four parameters that define the crush force profile (area, peak force, Gompertz function A, Gompertz function B), together with the kernel weight, were applied to a multiple linear regression equation. Given the large number of calibration samples, all five terms were included in the regression. The fitted versus actual yield had a significant but low correlation ($r^2 = 0.25$) with a residual standard deviation (RSD) of 1.5%. Figure 6 shows the corresponding scatter plot that exhibits a considerable amount of scatter about the fitted line. The repeatability of Buhler test milling (RSD 0.59%) when measuring SY% is better than the prediction model. The 99% confidence range for Buhler semolina milling is 1.77, and the range typically found for

milling durum in the Tamworth breeding program is 66.4–71.9%. Therefore, the error in the milling method represents about one third of the total variation in actual yields. The criteria for the usefulness of the SKCS SY% prediction in a breeding program depends on the percentage of incorrectly discarded or retained samples. Examination of the scatter diagram indicates that the application of a conservative cut-off value of 67.0% for SY% using the SKCS fitted yield data would have resulted in a total of 33 lines being discarded, of which 13 had actual yields >67% and would therefore have been incorrectly discarded. Conversely, 551 lines would be accepted and of these, 61 would have actual yields of <67% (11% poor yield lines accepted). The objective in breeding for improved grain quality is to move the population mean in the required direction, higher in the case of SY%. Despite the poor predictive ability, the SKCS method appears to have the potential to achieve this.

One of the main difficulties in predicting SY% in a breeding program at the early generation stage is the effect of environment on mill extraction. A cultivar or breeding line can display a wide range in mill yield across environments (Fig. 7). Some lines displayed a narrow range in SY% but others had quite a wide range, and on the basis of a causal relationship, they seemed to be related to the range in grain weight in these lines (30–57 mg in some cases). Because there is a positive correlation between SK-WT and SY% (Table V), this would account for some of the variation observed. Therefore, even if a line were tested by the SKCS 4100 at an early generation and predicted to have a low yield, that line progressing through the various generations could display a wide range in mill performance reflected in between-site and seasonal variation. Some lines may have a narrow range in SY% across environments, so these would be easier to predict. Attempts were made to obtain a prediction of SY% of advanced generation lines by analyzing the F3 seed from which these lines were derived. Although there was a significant correlation between predicted SY% on F3 lines and the Buhler SY% averaged across sites for F3-derived advanced lines ($r^2 = 0.18$, $P < 0.01$), the utility of that prediction is questionable. For example, if all lines below a SY% of 68 were rejected, many lines that performed above this SY% at some sites would also have been rejected. This is because some advanced lines varied considerably in their SY% across environments (by as much as 7.5% in one case) (Fig. 7). The environmental effect on SY% makes prediction in early generations uncertain. Further research will be conducted in an attempt to improve the value of the SKCS 4100 in the prediction of SY% for early generation screening.

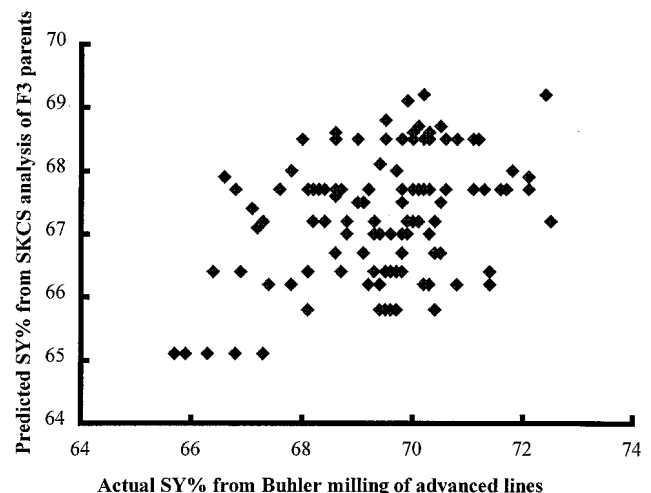


Fig. 7. Plot of single-kernel characterization system (SKCS) predicted semolina mill yield (SY%) by analysis of F3 parents against actual laboratory milled % semolina yield of advanced lines grown at various sites.

CONCLUSIONS

The application of the SKCS 4100 to the analysis of durum wheat in a breeding program has been studied. The instrument provides accurate and reliable data after adjustment of the factory-installed common wheat calibrations and replaces the more time-consuming 1,000 kernel weight and pearlograph hardness measurements previously used in the program. The SKCS 4100 generates information on sample uniformity that has yet to find use in a breeding program. The raw SKCS data can be used to develop a calibration for semolina mill yield, which could be useful for breeders to move the population mean to a higher semolina mill yield by screening out a proportion of the poorer lines. A calibration for durum vitreousness provides a more rapid and objective method than the visual inspection method.

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