

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

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### ABSTRACT

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Single-kernel characterization system (SKCS) 4100 measurements on wheat were reproducible and stable and gave good correlations with relevant reference data, e.g., kernel weight vs. 1,000 kernel weight, kernel hardness vs. particle size index, and kernel moisture vs. oven moisture. Under field conditions at a receiving station in Coleambally (NSW, Australia), the SKCS 4100 operated faultlessly and the reproducibility of the results was as good as in the laboratory. The measurements were completed within the time taken for the normal testing sequence, and the histograms were shown to provide valuable information about the samples that would not otherwise be available. For example, the distribution

of moisture contents of individual kernels provides additional information about the samples' potential storage stability. Data on the uniformity of hardness could be interpreted in terms of the potential of the wheat to provide a consistent milling performance. An imprecise ( $r^2 = 0.44$ ) but potentially useful calibration was obtained for the prediction of flour yield under test milling conditions using SKCS 4100 measurements on wheat. A much stronger correlation ( $r^2 = 0.83$ ) was obtained between SKCS data on wheat and the starch damage contents of flours produced on a pilot mill. Thus, the SKCS 4100 has the potential for early generation screening of wheat lines for flour yield and starch damage.

The single-kernel characterization system (SKCS) 4100 (Perten Instruments North America Inc., Reno, NV) was developed to provide an automated objective means of classifying wheat into U.S. grades (Martin et al 1993). The sample is deposited into a hopper where a rotating wheel (the singulator) picks up individual kernels with the aid of a vacuum and deposits them one at a time into a weighing boat then down an inclined crescent where the diameter is measured and the kernel is crushed between the crescent and a toothed rotor. A load cell measures and records the crush force profile. Simultaneously, the conductivity of the crushed kernel is measured. In normal operation, this sequence of operations is carried out automatically on each of a preset number (usually 300) kernels in a total test time of 3-5 min. In the course of the test, the SKCS 4100 computer collects 40 raw measurements from which kernel weight, diameter, hardness index, and moisture content are calculated using predetermined calibration equations and provides an objective classification as hard, soft, or mixed. At the end of the test, the distributions of kernel weights, diameters, hardness indices, and moisture contents for the grains in the sample are presented graphically and the results summarized as means and standard deviations for each of the four properties.

Assessment of grain samples for uniformity in terms of kernel weight, diameter, hardness, and moisture has great potential for improving wheat grading at receiving silos. Furthermore, because the SKCS 4100 test is rapid, simple, and requires a relatively small quantity of sample, it has the potential to provide information that could assist plant breeders to screen lines for quality at an earlier stage and at a lower cost than is currently possible. Results of recent studies have also indicated that calibration equations may be derived to predict additional quality characteristics from SKCS 4100 data including a direct measure of wheat kernel texture (Gaines et al 1996) and flour yield (Satumbaga et al 1995). Because there is a direct causal relationship between wheat kernel texture and flour starch damage potential, it might be envisaged that the latter could also be predicted from SKCS 4100 data. Therefore, the aims of this work were to evaluate the performance

of the SKCS 4100 for testing the uniformity of wheat at receiving silos and investigate its potential applications in breeding programs with particular reference to flour yield and starch damage.

### MATERIALS AND METHODS

A systematic evaluation of the potential applications of the SKCS 4100 was carried out as follows: 1) the repeatability and reproducibility of each of the SKCS 4100 test results was determined by replicate tests and analyses of variance, 2) the accuracy of each test result was evaluated by comparisons with standard methods, 3) the capabilities of the instrument were established by examining a range of genetically diverse wheats and by varying the numbers of kernels tested, 4) the potential applicability of the SKCS 4100 to receiving testing was evaluated by means of field trials, and 5) potential new applications to early generation quality screening in wheat breeding programs were studied.

#### Samples

Five sets of wheat samples were used in this study. Set one was used to assess the accuracy of SKCS 4100 moisture values. It comprised 35 samples with moisture contents ranging from 10.0 to 16.0%. These were prepared from five wheat samples (6 kg) as follows. Each wheat sample was cleaned using a Carter-Day dockage tester then divided into seven aliquots of 500 g. The moisture content of each sample was determined by near-infrared reflectance and the amount of water required to increase the moisture contents of the samples in 0.5% increments to 16.0% was calculated. The required amount of water by volume was added to the wheat in a plastic container with a screw cap. The cap was sealed and the container was rotated for 5 min so that the water was dispersed evenly over the surface of the wheat. The tempered wheat was stored overnight. The SKCS 4100 and oven moisture contents by AACC Method 44-15A (AACC 1995) were determined on the equilibrated samples on the same day.

Set two comprised 70 samples of wheats that had been in storage at constant temperature for some years. This set represented a collection of genetically diverse wheats of contrasting morphology ranging from shot wheats (*Triticum sphaerococcum* Percival) with essentially round grains to durum (*T. durum* Desfontaines) with long grains. This set also included wheat cultivars with extremes of hardness and covered spelt wheat (*T. spelta* L.). These samples were examined to evaluate the limits of application of the SKCS 4100.

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Set three comprised 150 wheat samples tested during receipt in December 1995 at a silo in Coleambally, New South Wales, Australia.

Set four comprised 32 samples of Australian Shipping Grades and some individual varieties collected over two growing seasons (1995 and 1996) to investigate the accuracy of SKCS weight compared with 1,000-kernel weight and of SKCS hardness index compared with particle size index (PSI) (Symes 1961). Selected samples were used to determine the repeatability and reproducibility of the SKCS 4100 measurements and to study the effect of number of kernels tested. The wheats were milled into straight-run flours using a 650 kg/hr pilot mill as described by Moss et al (1991) and the starch damage contents of the flours were determined by AACC Method 76-31 (AACC 1995).

Set five comprised samples from a soft wheat breeding program in Narrabri, New South Wales, Australia. This program was established to develop a stem, leaf, and stripe rust resistant derivative of the club wheat variety Tincurrin, which had high grain yield and good soft wheat quality for cookie production but was unsuitable for commercial production because of a susceptibility to rust. F<sub>5</sub> lines derived from three complex crosses designed to introduce stem, leaf, and stripe rust resistances into Tincurrin were planted in the 1995 season at two locations. Prior to harvest, all plots were rated for acceptable plant height, straw strength, uniformity, and potential yield. Only plots that rated highly on all counts and were resistant to all three wheat rusts were harvested, resulting in 561 grain samples. Grain was cleaned before conducting quality tests. Grain samples were equilibrated from variable harvest moisture contents ranging from 9–11% to approximately 12.5% moisture content in a preconditioning cabinet. The preconditioning regime involved storing the samples in paper bags for at least three weeks in racks within the cabinet and suspended

over a tray of super-saturated sodium nitrite solution at a constant temperature of 20°C. A 100-g grain sample was then milled to flour using a Quadrumat Junior flour mill fitted with a 0.28-mm silk screen. Flour yield was expressed on a total products basis as a percentage of conditioned wheat to first break.

### Single-Kernel Characterization System

SKCS 4100 measurements were carried out, using 300 grains unless otherwise specified, according to the operational manual (Perten Instruments 1995). The means and standard deviations for weight, diameter, hardness index, and moisture were recorded for all samples studied. Additionally, for sample sets four and five, a computer file containing the averages of 40 low-level machine variables was stored. These variables are listed in Table I. The primary variables were weight (mg), peak force (maximum load cell force, A/D count), conductivity (A/D count), area (area of the force crush 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 force-time crush profile), GompB (Gompertz function 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), moisture (%), XCON (conductance × unit thickness mm), crescent temperature (°F) and DyFraction (time interval that a kernel exerts force on the crescent). The remaining variables are derived from these primary variables.

### Statistical Analysis

All statistical analyses were conducted with MINITAB. Repeatability and reproducibility were calculated by analysis of variance on data from three samples tested by three different operators on three different days. Simple correlations between standard and SKCS 4100 data were calculated using the method of least squares. Equations for the prediction of flour yield and starch damage were derived using all 40 low-level machine variables (Table I). Because many of the data are intercorrelated, principal components analysis was performed prior to multiple regression analysis.

## RESULTS AND DISCUSSION

### Measurement Precision and Accuracy

There was no significant effect ( $P > 0.05$ ) on the mean SKCS weight, diameter, hardness index, or moisture values among operators on three different days. The pooled standard deviations of

TABLE I  
Single-Kernel Characterization System (SKCS) 4100 Low-Level Machine Variables

| Variable Number | Description <sup>a</sup> | Variable Number | Description                  |
|-----------------|--------------------------|-----------------|------------------------------|
| 1               | Kernel Weight            | 21              | (Kernel Weight) <sup>2</sup> |
| 2               | Peak Force               | 22              | 1/(Kernel Weight)            |
| 3               | Conductivity             | 23              | (Gomp B) <sup>7</sup>        |
| 4               | Area                     | 24              | (Gomp B) <sup>8</sup>        |
| 5               | Gomp A                   | 25              | (Gomp B) <sup>10</sup>       |
| 6               | Gomp B                   | 26              | DyFraction 5–10              |
| 7               | Crush Length             | 27              | DyFraction 10–15             |
| 8               | Moisture                 | 28              | DyFraction 15–20             |
| 9               | XCON                     | 29              | DyFraction 25–30             |
|                 | (Conductivity*gap)       |                 |                              |
| 10              | Temperature (Crescent)   | 30              | 1/(Peak Force)               |
| 11              | Temperature <sup>2</sup> | 31              | √area                        |
| 12              | In(Temperature)          | 32              | √Kernel Weight               |
| 13              | In(XCON)                 | 33              | Area*XCON                    |
| 14              | 1/XCON                   | 34              | √(Area*XCON)                 |
| 15              | In(Temp)*In(Area)        | 35              | In(Area)*In(XCON)            |
| 16              | (Gomp B) <sup>9</sup>    | 36              | (Gomp B) <sup>9</sup> *XCON  |
| 17              | DyFraction 20–25         | 37              | Peak Force*XCON              |
| 18              | In(Area)                 | 38              | Peak Force*In(XCON)          |
| 19              | In(Kernel Weight)        | 39              | Peak Force*Crush Length      |
| 20              | In(Moisture)*In(Temp.)   | 40              | √(In Kernel Weight))         |

<sup>a</sup> Weight measured in mg, peak force (maximum load cell force, A/D count), conductivity (A/D count), area (area of the force crush 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 force-time crush profile), GompB (Gompertz function 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), moisture (%), XCON (conductance × unit thickness mm), crescent temperature (°F) and DyFraction (time interval that a kernel exerts force on the crescent).

TABLE II  
Results of ANOVA for Single-Kernel Characterization System (SKCS) 4100 Test Results

| Measurement  | σ <sub>F</sub> | σ <sub>R</sub> |
|--------------|----------------|----------------|
| Weight, mg   | 0.65           | 0.74           |
| Diameter, mm | 0.029          | 0.040          |
| Hardness     | 0.90           | 1.37           |
| Moisture, %  | 0.036          | 0.22           |

TABLE III  
Results of Regression of Standard Analytical Data on Single-Kernel Characterization System (SKCS) 4100 Data

| Regression Variables |                  | Range of y-variable | Correlation Coefficient | RSD <sup>a</sup> |
|----------------------|------------------|---------------------|-------------------------|------------------|
| x                    | y                |                     |                         |                  |
| Weight               | 1,000 kernel wt  | 31.0–39.0 g         | 0.970                   | 0.5 g            |
| Moisture             | Oven moisture    | 10.0–12.5%          | 0.983                   | 0.32%            |
| Hardness             | PSI <sup>b</sup> | 8–24%               | -0.785                  | 2.6%             |

<sup>a</sup> Residual standard deviation.

<sup>b</sup> Particle size index.

repeatability ( $\sigma_r$ ) and reproducibility ( $\sigma_R$ ) for each of the four measurements are given in Table II. When expressed as coefficients of variation, these are in the range 1.5–2.0%, which may be considered excellent. It should be noted that, by definition, reproducibility includes between-laboratory variance. In this case however, because only one instrument was available, the “reproducibility” represents different operators, days, and subsamples but not different laboratories. The accuracies of the SKCS weight and moisture results as assessed against standard methods were also satisfactory (Table III). There was a satisfactory correlation between SKCS hardness index and hardness measured by the PSI method (Table III).

### Capabilities of the Instrument

Sets of 6, 12, 25, 50, 100, 200, 300, and 400 grains of three samples were tested using the SKCS 4100. The mean and standard deviation of each set of data were compared for each number of grains tested to ascertain the minimum sample size that results in a consistent mean and low standard deviation. Fig. 1 shows that, over the four test results for the three samples, the SKCS 4100 can produce satisfactory results using as few as 50 grains (i.e., approximately 2 g of wheat). However, measurements on fewer grains lead to fluctuations in the mean and increases in the standard deviation of the measurements. The ability to perform the test using only 2 g of wheat would be a significant advantage in situations where sample size is limited. In particular, it might be envisaged that it would enable breeding lines to be tested for quality as early as the F<sub>2</sub> generation rather than at F<sub>4</sub>–F<sub>6</sub>.

Samples ranging from soft wheats with essentially round grains (SKCS mean diameter = 2.76 mm, standard deviation [SD] = 0.53 mm) to durum with long grains (SKCS mean diameter = 2.93 mm, SD = 0.03 mm) fed with equal ease through the instrument. A covered spelt wheat (SKCS mean diameter = 2.25 mm, SD = 0.41 mm) could also be tested without difficulty. A range of old Australian varieties that included wheat softer (e.g., Mentona; SKCS mean hardness index = 33.1, SD = 12.6) and harder (e.g., Baringa; SKCS mean hardness index = 99.9, SD = 12.3) than any currently

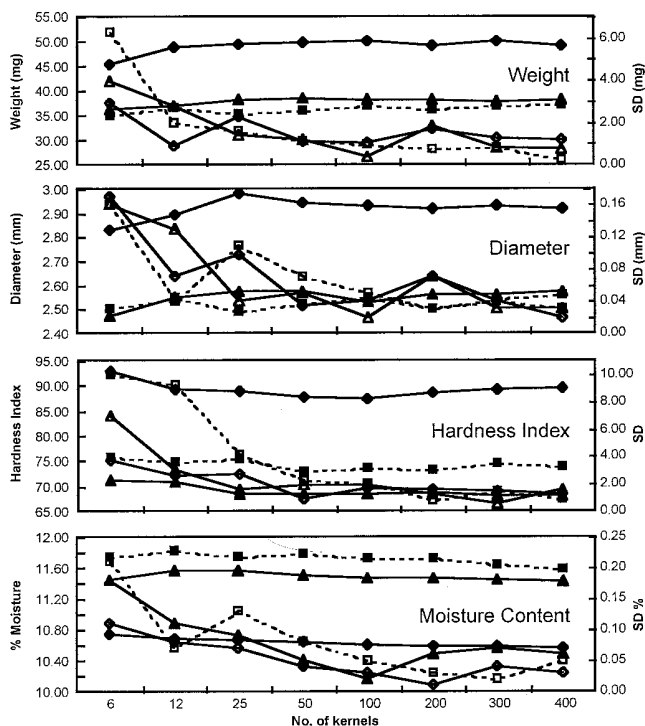


Fig. 1. Comparison of single-kernel characterization system weight, diameter, hardness index, and moisture content of three different grains.  $\blacktriangle$  = Suneca,  $\blacksquare$  = Trident, and  $\blacklozenge$  = durum (open symbols are standard deviations).

in cultivation produced results consistent with their known properties. Furthermore, this set of wheats, which had been in storage at constant temperature for some years, resulted, as expected, in histograms that showed a very narrow range of moisture (SD as low as 0.16%).

### Field Trials

The SKCS 4100 is applicable to the classification of wheat at receiving stations. Therefore, one of the aims of the project was to evaluate the potential application of this instrument for checking the grade and uniformity of wheat received in Australia. Although the SKCS 4100 had performed well in the research laboratory, this aim could not be truly evaluated without extending the evaluation to an actual receiving station. Therefore, field trials were arranged for a short period of time in December 1995 at the Coleambally wheat silo, New South Wales, Australia. The Coleambally site was chosen on the basis that a wide variety of wheats of varying hardness and grown under both irrigated and dryland production situations are received there.

In total, 150 samples were tested, 64 of which were duplicates. During the period of the field trials, the Coleambally silo received wheat deliveries representing the Australian wheat grades Australian soft, Australian standard white, and Australian hard. Hectoli-

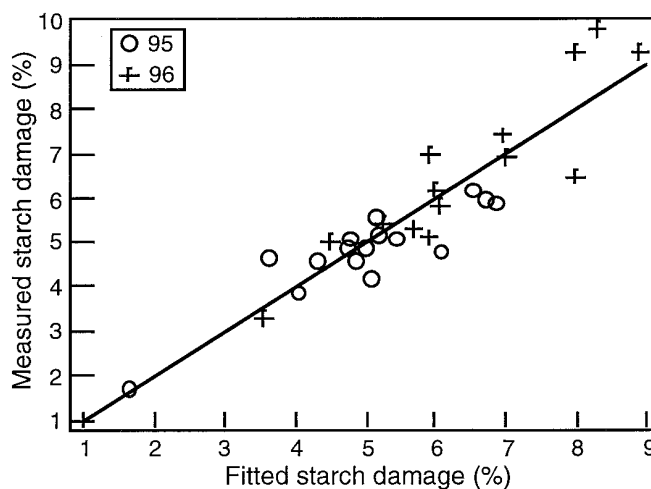


Fig. 2. Plot of measured versus fitted starch damage using 10 principal components calculated from single-kernel characterization system (SKCS) 4100 low-level machine data; data from 1995 (95) and 1996 (96) crop years combined.

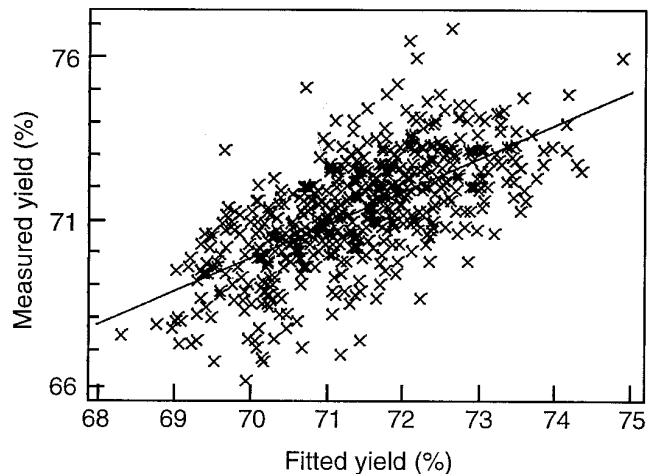
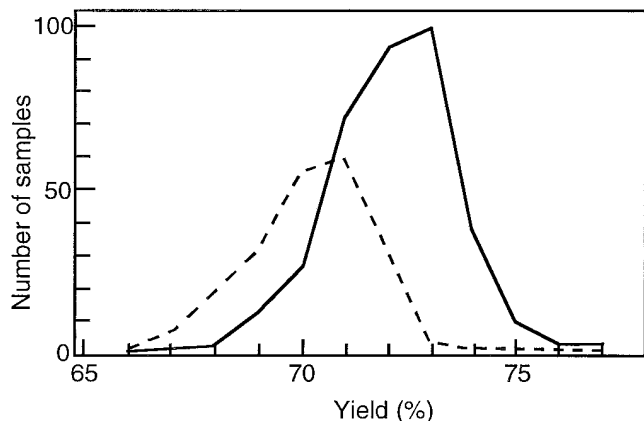


Fig. 3. Plot of measured versus fitted flour yield using 10 principal components calculated from single-kernel characterization system (SKCS) 4100 low-level machine data.



**Fig. 4.** Histogram of Brabender flour yields for wheat breeding lines rejected (dotted line) and selected (solid line) on the basis of a cutoff of 71% using single-kernel characterization system (SKCS) 4100 predicted flour yield values.

ter weights ranged from 74.5 to 85.5 kg/hL, and moisture contents ranged from 8.5 to 12.0%. The measurements were carried out according to the test method previously established and no modifications to the method were required. The SKCS results on received samples were obtained within the normal testing cycle, which was at the rate of 12 to 15 truckloads per hour. With appropriate daily maintenance (Perten Instruments 1995), the SKCS 4100 operated faultlessly and the results obtained on check samples remained within control limits (set at  $\pm 3\sigma_R$ ) throughout the trials in a sampling shed that was not air conditioned and where the ambient temperature ranged between 24 and 35°C, the instrument and crescent temperatures reached 33.9 and 40.1°C, respectively. The air filter appeared to have a greater build-up of dust particles than usual, but it is to be expected that replacement of the filter would need to be more frequent in wheat receiving stations than in research laboratories. This study has provided a demonstration of the potential value of the SKCS 4100 in grain segregation in Australia.

#### Potential New Applications

A multiple linear regression equation was derived for predicting starch damage on straight-run pilot-milled flour from the first 10 principal components calculated from the SKCS 4100 low-level machine data on the 32 parent wheats. The choice of 10 principal components was made before examining the regression, on the arbitrary basis that they accounted for 99.9% of the variance in the low-level machine data. The equation had an  $r^2$  of 0.83 and a residual standard deviation of 0.88%. Data from both seasons were included in the same calibration. The corresponding scatter plot with the 1995 and 1996 data distinguished is shown in Fig. 2. While this calibration needs to be verified using further samples, the result is sufficiently encouraging to suggest that potential exists for SKCS 4100 measurements to predict flour starch damage. The level of starch damage of a flour sample, together with its protein and moisture contents, controls the water absorption. Adjustment of reduction roll pressures to control starch damage is the means by which a target flour water absorption is achieved from a wheat of given protein content. The potential of a wheat cultivar to produce a high level of starch damage for a given roll pressure is an important characteristic when selecting lines for breadmaking quality.

A multiple linear regression equation was derived for predicting flour yield from the first 10 principal components calculated from low level machine data on the 561 wheat breeding lines. The equation had an  $r^2$  of 0.44 and a residual standard deviation of 1.3%. Fig. 3 shows the corresponding scatter plot, which confirms

that although there is a significant relationship between flour yield and SKCS data, there is also a considerable amount of scatter about the fitted line. Tincurrin samples milled as controls had a mean flour yield of 71.8% ( $n = 22$ ). Examination of the scatter diagram (Fig. 3) indicates that application of a conservative cut-off value of 71% based on the SKCS 4100 data would have resulted in some lines with high flour yield being discarded and conversely, some with poor flour yield being retained. However, breeders would be more inclined to err on the conservative side with an early generation test. This means minimizing the proportion of lines incorrectly discarded (i.e., those in the upper left quadrant of Fig. 3 above the coordinates 71, 71). In fact, only a very few of the total number of lines under evaluation fall into this quadrant and would therefore have been incorrectly discarded.

Because the objective was to determine whether the SKCS 4100 has the potential to segregate breeding lines according to flour yield, it was of interest to examine the data in a different way. Fig. 4 illustrates the effect of selecting from this particular set of breeding lines on the basis of flour yield as predicted by the SKCS 4100. If an arbitrary flour yield cutoff of 71% were chosen, 355 samples would be selected and 206 rejected. The diagram shows the measured Brabender flour yields for the selected and rejected samples and confirms that almost all lines with flour yields less than 68%, but almost none of the lines with flour yields greater than 73% were rejected.

#### CONCLUSIONS

A test method based on the SKCS 4100 has been shown to produce accurate and reproducible measurements of kernel weight, diameter, hardness, and moisture content on as few as 50 individual kernels of wheat. The SKCS 4100 generates information on sample uniformity not otherwise available. The SKCS 4100 is sufficiently robust and rapid for use at grain receiving silos. The raw SKCS data offer the potential to screen early generation plant breeding lines for milling and flour quality.

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