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Modelling wheat breakage during roller milling using the Double Normalised Kumaraswamy Breakage Function: Effects of kernel shape and hardness

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ABSTRACT

The effects of wheat properties on breakage during First Break roller milling, as described by the Double Normalised Kumaraswamy Breakage Function (DNKBF), were investigated. A set of 45 wheats from nine varieties representing the range of commercial varieties grown in the UK, and grown over three harvest years at several nitrogen fertiliser levels, were milled at five roll gaps under Sharp-to-Sharp and Dull-to-Dull dispositions. The resulting particle size distributions were fitted with a DNKBF in order to understand the physical significance of the DNKBF parameters and to relate them to shape and hardness. The DNKBF parameters related strongly to hardness as measured using either the Single Kernel Characterisation System or Particle Size Index, allowing the particle size distribution over the range 0–4000 μm to be predicted solely from wheat hardness. A residual analysis showed that the remaining variation was correlated with kernel mass, and that more elongated kernels break to give slightly larger particles than more spherical kernels of equivalent hardness. Two types of breakage are identified, one of which principally produces many small endosperm particles along with large bran particles, while the other tends to produce mid-sized particles. The former dominates under Dull-to-Dull milling and for soft wheats, while the latter becomes more prominent under Sharp-to-Sharp milling and for harder wheats.

1. Introduction

The particle size distribution produced during First Break roller milling of wheat is a critical control point in the flour milling process (Campbell et al., 2007; Hsieh et al., 1980), and is also relevant to the fractionation and further processing of wheat for non-food uses in biorefineries (Campbell, 2007; Mateos-Salvador et al., 2011). Wheat breakage depends on the design and operation of the roller mill and on the properties of the wheat, specifically the distributions of kernel characteristics such as size, hardness and shape (Campbell and Webb, 2001, 2007). These distributions can be characterised using the Perten Single Kernel Characterisation System (SKCS, Perten Instruments, Sweden), which crushes 300 kernels within 5 min and reports the distributions of their mass, diameter, hardness and moisture content (Martin et al., 1991, 1993; Martin and Steele, 1996; Osborne and Anderssen, 2003). Hardness as measured by the SKCS has proved to be a useful and meaningful measure, but the basis of its calculation using a commercially secret algorithm is not fully known (Osborne and Anderssen, 2003). The breakage equation was introduced to relate these distributions of single kernel properties to the outlet particle size distribution (psd) resulting from First Break milling (Campbell and Webb, 2001, 2007). Recently, Mateos-Salvador et al. (2011) introduced a new form of the breakage function, the Normalised Kumaraswamy Breakage Function (NKBF), as a more practical and meaningful alternative to the original polynomial breakage functions. However, the NKBF was tested on a limited sample set, such that effects of kernel properties on the parameters of the NKBF could not be identified unambiguously. Therefore the objectives of the current work were to investigate the effects of kernel hardness and shape on NKBF parameters, to understand the physical significance of NKBF parameters, and to extend the NKBF to allow predictions of breakage to be made directly from SKCS data.

Abbreviations: DNKBF, Double Normalised Kumaraswamy Breakage Function; D–D, Dull-to-Dull; S–S, Sharp-to-Sharp; psd, particle size distribution; SKCS, Single Kernel Characterisation System; PSI, Particle Size Index.

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2. The Normalised Kumaraswamy Breakage Function

The Kumaraswamy equation, as applied to First Break roller milling of wheat, is:

$$p_2(z) = (1 - P_{\min}) m n z^{m-1} (1 - z^m)^{n-1} \quad (1)$$

Integrating Eq. (1) gives the cumulative distribution function form:

$$P_2(z) = P_{\min} + (1 - P_{\min})\left(1 - (1 - z^m)^n\right) \quad (2)$$

where $P_2(z)$ and $p_2(z)$ are the cumulative and non-cumulative probability distributions, respectively, of the independent variable, z. The independent variable must lie in the interval [0,1]. $P_{\min}$ is the cumulative probability corresponding to the minimum particle size, $x_{\min}$. In the current work, $x_{\min}$ and $P_{\min}$ are always zero, but their inclusion allows for a general definition applicable to cases when the minimum particle size is not zero. m and n are shape parameters, which have positive values. For application to wheat milling, the independent variable, which normalises the data obtained using different roll gaps, was defined by Mateos-Salvador et al. (2011) as:

$$z = \frac{\chi}{\chi_{\max}} \quad (3)$$

$$\chi = \frac{x - x_{\min}}{(G/D)^a} \quad (4)$$

where G is the roll gap and D the average wheat kernel size, such that G/D forms the milling ratio, and a is the collapsing parameter that normalises data from different milling ratios to fall onto the same curve. χ is therefore the normalised particle size, while $\chi_{\max}$ is given by the maximum measured particle size and the minimum milling ratio used to generate the data.

Mateos-Salvador et al. (2011) used the NKBF to re-examine the experimental data of Campbell et al. (2007). The coefficient of determination, when fitting this data using the NKBF, varied between 0.977 and 0.994. Although these values are lower than those obtained using the original polynomial breakage function, which gave values greater than 0.990 for the same dataset due to its

Table 1
Wheat samples used in the study, their average kernel properties as measured by the Single Kernel Characterisation System (SKCS), and their hardness as indicated by Particle Size Index.

Wheat type	Sample no.	Nitrogen application rate (kg/ha)	Harvest year	SKCS hardness (arbitrary units)	Mass (mg)	Diameter (mm)	Shape factor (mg/mm^3)	PSI hardness (arbitrary units)
Avalon	1	200	2006	58.10	50.08	3.04	1.78	11.68
	2	100	2007	39.34	51.96	3.20	1.59	15.59
	3	200	2007	41.07	53.08	3.22	1.59	14.16
	4	350	2007	41.65	51.26	3.11	1.70	11.96
	5	200	2008	43.94	55.64	3.27	1.59	12.20
Beaver	6	200	2006	31.87	38.19	2.82	1.70	20.19
	7	100	2007	14.36	44.94	3.07	1.55	24.24
	8	200	2007	13.35	48.22	3.11	1.60	19.95
	9	350	2007	15.51	47.48	3.09	1.61	18.20
	10	200	2008	13.29	50.47	3.20	1.54	20.04
Cadenza	11	200	2006	78.17	41.62	2.90	1.71	9.71
	12	100	2007	42.96	53.88	3.40	1.37	13.49
	13	200	2007	60.18	50.83	3.27	1.45	9.55
	14	350	2007	63.58	49.71	3.22	1.49	8.75
	15	200	2008	63.80	51.54	3.33	1.40	11.91
Claire	16	200	2006	32.97	40.91	2.85	1.77	13.77
	17	100	2007	14.04	46.43	3.11	1.54	19.02
	18	200	2007	19.52	45.74	3.06	1.60	17.69
	19	350	2007	23.97	44.41	3.03	1.60	16.12
	20	200	2008	16.48	51.53	3.25	1.50	18.96
Hereward	21	200	2006	60.38	42.18	2.95	1.64	10.38
	22	100	2007	35.64	47.68	3.22	1.43	15.17
	23	200	2007	40.50	45.96	3.16	1.46	13.18
	24	350	2007	47.06	42.34	3.03	1.52	10.97
	25	200	2008	41.58	50.59	3.31	1.40	11.28
Istabraq	26	200	2006	23.57	47.57	3.04	1.69	17.43
	27	100	2007	6.74	48.59	3.18	1.51	20.29
	28	200	2007	17.16	47.45	3.12	1.56	18.78
	29	350	2007	16.82	45.72	3.09	1.55	17.61
	30	200	2008	14.44	46.49	3.12	1.53	20.00
Malacca	31	200	2006	65.73	36.96	2.87	1.56	10.93
	32	100	2007	45.63	45.92	3.24	1.35	13.13
	33	200	2007	50.81	48.98	3.33	1.33	11.53
	34	350	2007	52.77	44.84	3.19	1.38	10.87
	35	200	2008	44.46	48.81	3.28	1.38	13.73
Riband	36	200	2006	31.64	45.90	3.08	1.57	19.20
	37	100	2007	13.98	48.91	3.29	1.37	19.85
	38	200	2007	18.30	46.42	3.19	1.43	18.56
	39	350	2007	17.91	48.52	3.23	1.44	10.23
	40	200	2008	20.69	53.27	3.33	1.44	–
Robigus	41	200	2006	36.27	39.37	2.85	1.70	16.03
	42	100	2007	19.84	42.54	3.05	1.50	19.26
	43	200	2007	22.76	39.54	2.92	1.59	15.41
	44	350	2007	18.89	42.28	3.00	1.57	15.48
	45	200	2008	16.37	46.46	3.08	1.59	–

larger number of parameters, the NKBF is considerably simpler, such that the slightly reduced accuracy of the fit is an acceptable price to pay.

Although the majority of the datasets used by Mateos-Salvador et al. (2011) were of incomplete particle size distributions, a further investigation was carried out into whether the NKBF is able to describe the complete psd. Using a single sample set, based on milling a sample of Alchemy wheat, Mateos-Salvador et al. (2011) concluded that it was possible to describe the entire psd over the range 0–4000 μm if the data was split into a fine range (0–2000 μm) and a coarse range (2000–4000 μm), with separate NKBF functions applied to each range. 2000 μm was chosen as an appropriate cut-off point between the coarse and fine ranges as it relates to commercial practice; the material that enters the Second Break in a commercial mill is usually that which is larger than 2000 μm.

In the current research, a single function that describes the entire particle size range from 0 to 4000 μm was investigated and appeared to describe wheat breakage well. Rather than divide the function into two separate ranges as Mateos-Salvador et al. (2011) suggested, a function named the Double NKBF was created that describes two types of breakage in parallel:

$$P_2(z) \equiv B(x,D) = \alpha \underbrace{\left(1-(1-z^{m_1})^{n_1}\right)}_{\text{Type 1 Breakage}} + (1-\alpha)\underbrace{\left(1-(1-z^{m_2})^{n_2}\right)}_{\text{Type 2 Breakage}} \tag{5}$$

where α is the proportion of the breakage that can be described as Type 1 breakage. m_1 and n_1 are parameters corresponding to Type 1 breakage; m_2 and n_2 are parameters corresponding to Type 2 breakage. The non-cumulative form of the DNKBF is:

$$p_2(z) = \alpha \underbrace{\left(m_1 n_1 z^{m_1-1}(1-z^{m_1})^{n_1-1}\right)}_{\text{Type 1 Breakage}} + (1-\alpha)\underbrace{\left(m_2 n_2 z^{m_2-1}(1-z^{m_2})^{n_2-1}\right)}_{\text{Type 2 Breakage}} \tag{6}$$

The advantages of the DNKBF over two NKBFs fitted separately to the fine and coarse ranges are that it avoids a separation at 2000 μm, and that it entails five instead of nine parameters to describe the breakage. A disadvantage is that it precludes separate values of the collapsing parameter a for the two size ranges. Mateos-Salvador et al. (2011) found differences in the collapsing parameter a for the coarse and fine ranges. However, the slight loss of accuracy may be an acceptable compromise for the enhanced simplicity. A further advantage of the proposed DNKBF is that it appears to reveal two types of breakage, called here Type 1 and Type 2 breakage, which may relate more directly to underlying physical factors contributing to breakage.

The application of the DNKBF was investigated in the current work for a large sample of wheats varying widely in kernel characteristics.

3. Materials and methods

A sample set of 45 wheat samples, representing the range of wheats commercially grown in the UK, was sourced from the Wheat Genetic Improvement Network (WGIN) nitrogen use field trials at Rothamsted Research (Barraclough et al., 2010). The samples consisted of nine wheat varieties (Table 1), covering a wide range of kernel hardness and shape, each grown at an intermediate nitrogen fertiliser level (200 kg/ha) over three harvest years (2006–2008) as well as the same nine wheats grown at three different nitrogen levels (100, 200 and 350 kg/ha) for one of the harvest years, 2007.

A 1 kg batch of each wheat was conditioned to 16% moisture (wet basis), then 100 g samples were milled at five roll gaps (0.3, 0.4, 0.5, 0.6 and 0.7 mm) on the Satake STR-100 test roller mill (Satake Corporation, Hiroshima, Japan), under both Sharp-to-Sharp (S–S) and Dull-to-Dull (D–D) roll dispositions, as described by Campbell et al. (2007). However, a slight difference of protocol was that, for practical reasons, the samples were allowed to condition for three days before milling, instead of overnight as practised by Campbell et al. (2007) and Mateos-Salvador et al. (2011); this may have affected their breakage patterns relative to this earlier work. The broken stocks were sieved on the Satake Laboratory Plansifter (Satake Corporation, Hiroshima, Japan), initially for 5 min on a coarse sieve stack with sizes 4000, 3550, 3350, 3150, 2800, 2500 and 2360 μm. The fraction ending on the pan was then sifted for a further 5 min on a fine sieve stack with aperture sizes 2000, 1700, 1400, 1180, 850, 500 and 212 μm. The mass of milled wheat remaining on each sieve within each stack was weighed using a Sartorius BP 610 balance to an accuracy of 0.005 g. Thus for each of the 45 wheats, a total of ten particle size distributions were obtained corresponding to five roll gaps under two roll dispositions.

For each wheat under each disposition, the five particle size distributions were collapsed, and the DNKBF fitted, using the Microsoft Excel Solver function to find the best fit values of a, α, m_1, n_1, m_2 and n_2. The variation of these parameters with kernel hardness and shape was then investigated.

Kernel characteristics were measured using the Single Kernel Characterisation System (SKCS Model 4100, Perten Instruments, Sweden). For each wheat, 300 kernels were processed in the SKCS, and the average hardness, mass, diameter and moisture content recorded. A shape factor was calculated as SKCS mass/diameter-cubed, on the rationale that for a given diameter and constant density, a larger mass ought to be indicative of a more elongated kernel. The assumption of relatively unvarying density was shown to be reasonable because shape factor was highly correlated with length:width ratio ($r^2 = 0.68$, results not shown), demonstrating that differences arose principally from shape.

Kernel hardness was also evaluated by measuring the psd in the fine flour fraction using a Coulter Lasersizer LS130. The proportion of particles in the size range 20–25 μm is different for hard and soft wheats (Devaux et al., 1998). The cumulative volume (% of total volume) of particles between 19.65 and 25.83 μm was determined. This value was called the Particle Size Index (PSI), and is reported in Table 1 (note, however, that insufficient sample prevented this analysis for two of the wheats).

4. Results and discussion

Table 1 lists the wheats and their corresponding SKCS characteristics after conditioning. The specific effects of harvest year and nitrogen level on grain properties are not the focus of the current paper; these wheats were selected from a larger trial that is the subject of a more comprehensive analysis elsewhere (Barraclough et al., 2010). For the purposes of the current work, the wheats serve to provide a sample set with a wide range of properties, in order to relate kernel properties to breakage, irrespective of the origin of the variation. Nevertheless, it is evident that wheats from the harvest year 2006 were, in general, noticeably harder, smaller and more elongated than from the subsequent two years. Higher levels of nitrogen application gave, in general, harder wheats (more so for harder than for softer varieties) that were smaller and more elongated. This is in accordance with studies performed by Lyon and Shelton (1999) who found that for kernels with an average hardness of 46, the effect of increasing nitrogen level was an increase in kernel hardness. Similarly, Shimshi and Kafkafi (1978) observed that increasing nitrogen fertiliser decreased wheat kernel mass, in agreement with the current observations.

The power of the breakage equation is to be able to take a sample of wheat, of unknown origin and history, possibly comprising a mixture of several wheats, and to predict its breakage based solely on the distributions of kernel characteristics as measured by the SKCS. Average kernel diameter, as reported by the SKCS, is incorporated within the milling ratio. It remains, therefore, to relate the NKBF shape parameters to the other SKCS parameters. Wheat is typically conditioned to 16% moisture content prior to milling, so accounting for the effect of moisture content is generally unnecessary (although can be done, as shown by Fang and Campbell, 2003b). Wheat hardness is the most critical factor affecting breakage and indeed wheat quality and functionality generally (Campbell, 2007; Pomeranz and Williams, 1990). Following the approach of Campbell et al. (2007), the relationship of the parameters of the DNKBF with SKCS hardness was investigated. A residual analysis was then performed to see if breakage patterns not predicted by hardness were related to kernel shape as indicated by SKCS mass/diameter-cubed.

Fig. 1(a) shows the variation with hardness of the fitted DNKBF parameter a, the collapsing parameter defined in Eq. (4) that

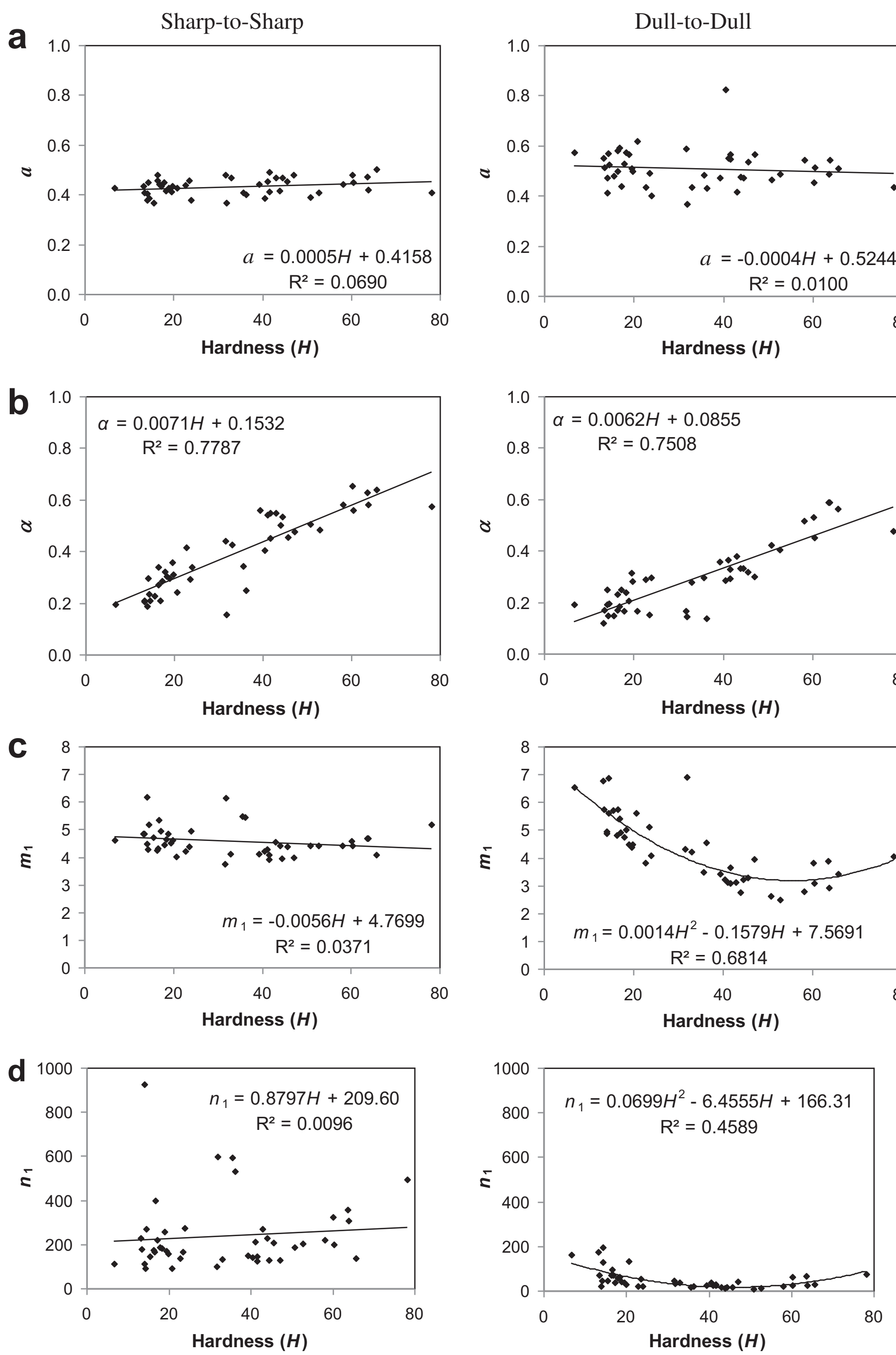

Fig. 1. Variation of collapsing parameter a and of Double NKBF parameters α, m_1, n_1, m_2 and n_2 with SCKS hardness under Sharp-to-Sharp and Dull-to-Dull milling.

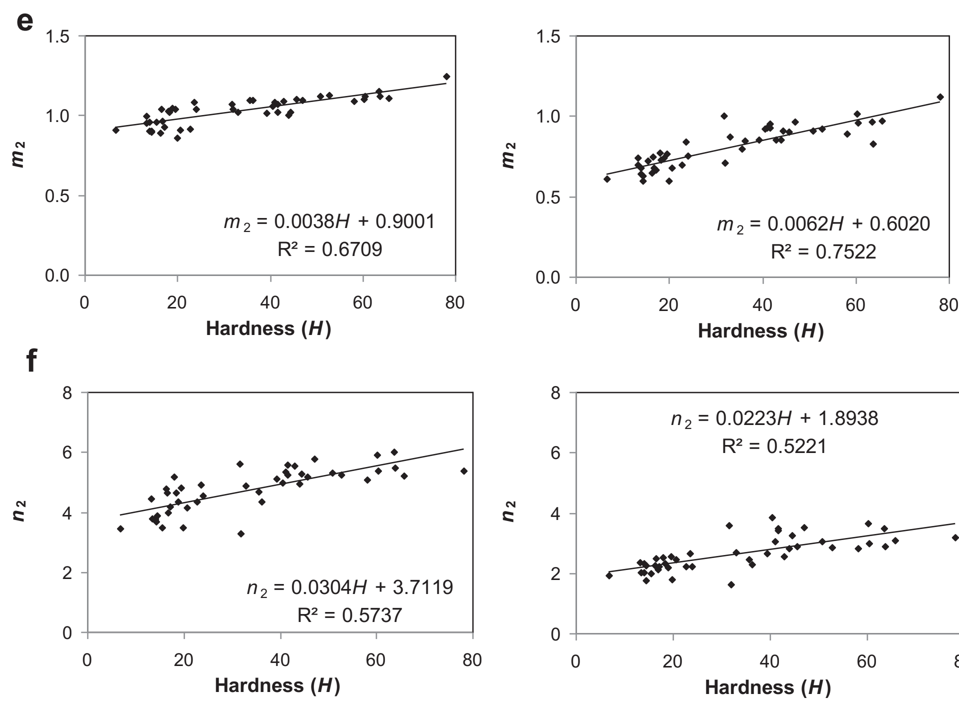

Fig. 1. (*continued*).

describes the response to changes in the milling ratio. Under both D–D and S–S dispositions there appears to be essentially no effect of hardness on the collapsing parameter; all wheats responded similarly to changes in the milling ratio. Interestingly, under a D–D disposition, parameter a exhibits a constant value of approximately 0.5, suggesting a square root relationship between output particle size and milling ratio (G/D) for all wheats. This may reflect the fundamental mechanics of breakage under this geometry. Under an S–S relationship, the parameter a exhibits a value closer to 0.4; this implies that breakage is less sensitive to milling ratio under S–S milling. Mateos-Salvador et al. (2011) similarly found an essentially constant value of a under S–S milling, at a slightly higher value of around 0.6, possibly reflecting in part the different conditioning time used in that work. However, they found a strongly negative correlation of a with hardness under D–D milling, in contrast with the essentially constant value found here. This is probably a result of fitting the full particle size range, which under D–D milling is more affected by large particles than under S–S milling. As noted above, a disadvantage of the DNKBF is that it obliges a constant value of a over the full size range, whereas Mateos-Salvador et al. (2011) found that different values of a may be appropriate for the smaller and larger ends of the psd; the production of small and large particles responds differently to changes in the milling ratio. Thus the constant value of 0.5 for a found here for D–D milling is between the two values applied separately to the coarse and fine ranges by Mateos-Salvador et al. (2011). In the case of S–S milling, there is very little coarse material (>2000 μm), so it has little influence on the value of a when fitting the DNKBF. The convenience of a single a parameter, combined with the further convenience of it having a constant value for all wheats, and the lesser practical importance of the precise psd of >2000 μm material with respect to the rest of the flour milling process, supports the use of the DNKBF as a practical and adequately accurate model.

It is appropriate at this point to introduce Fig. 2 to show the collapsed data and corresponding DNKBF fits for three illustrative wheats under both S–S and D–D milling. The three wheats have been selected to illustrate fits of the best, worst and intermediate quality, as indicated by the R^2 values, and also to represent wheats of different hardness. All three wheats are from the 2007 harvest and grown at an intermediate nitrogen level of 200 kg/ha. The Cadenza sample is a moderately hard wheat (hardness index = 60.2) for which the data from the different roll gaps collapsed well onto a single curve under both S–S and D–D dispositions. The Hereward sample (hardness index = 40.5) was the softest of the four “hard” breadmaking wheats (the others being Avalon and Malacca) and gave the poorest collapse of all the wheats under D–D, although one of the best under S–S. Istabraq was the softest of all of the wheats (hardness index = 17.2) and collapsed moderately well under D–D.

The S–S curves are more to the left than the corresponding D–D curves in Fig. 2, implying on average smaller particles. They are also steeper in the middle, implying a greater proportion of mid-sized particles under S–S compared with D–D, in agreement with previous findings (Campbell, 2007; Campbell et al., 2007). In general, it is clear that the data generated by S–S milling collapsed very well when transformed using Eq. (4) and the collapsing parameter a. The data generated by D–D milling in general collapsed less well. This is because these data were more influenced by larger particles; D–D milling results in a greater proportion of large particles than S–S milling, as is evident from Fig. 2, and creation of these large particles may respond to changes in milling ratio differently to small particles. Thus, arguably, the approach of Mateos-Salvador et al. (2011) to collapse fine and coarse data separately should be applied to D–D milling. However, the benefits of the DNKBF with its single collapsing parameter are sufficient, and the collapses adequate, to pursue this approach further.

A benefit of the DNKBF is that, when it fits the data well, it suggests that there are two predominant breakage mechanisms occurring simultaneously, which we have named here Type 1 and Type 2 breakage. The parameter α determines the balance between these two types of breakage. Fig. 1(b) shows the effect of hardness on α. Clearly, under both S–S and D–D milling, the proportion of Type 1 breakage increased with hardness (Note that, for 45 data points, an R^2 value >0.216 is statistically significant at $p < 0.001$.). Under both dispositions, Type 2 breakage dominates for soft wheats, while the contributions from the two types of breakage become more equal for harder wheats.

Fig. 2(b) illustrates the breakage for the three wheats used in Fig. 2(a), showing the best fit Type 1 and Type 2 breakage curves in

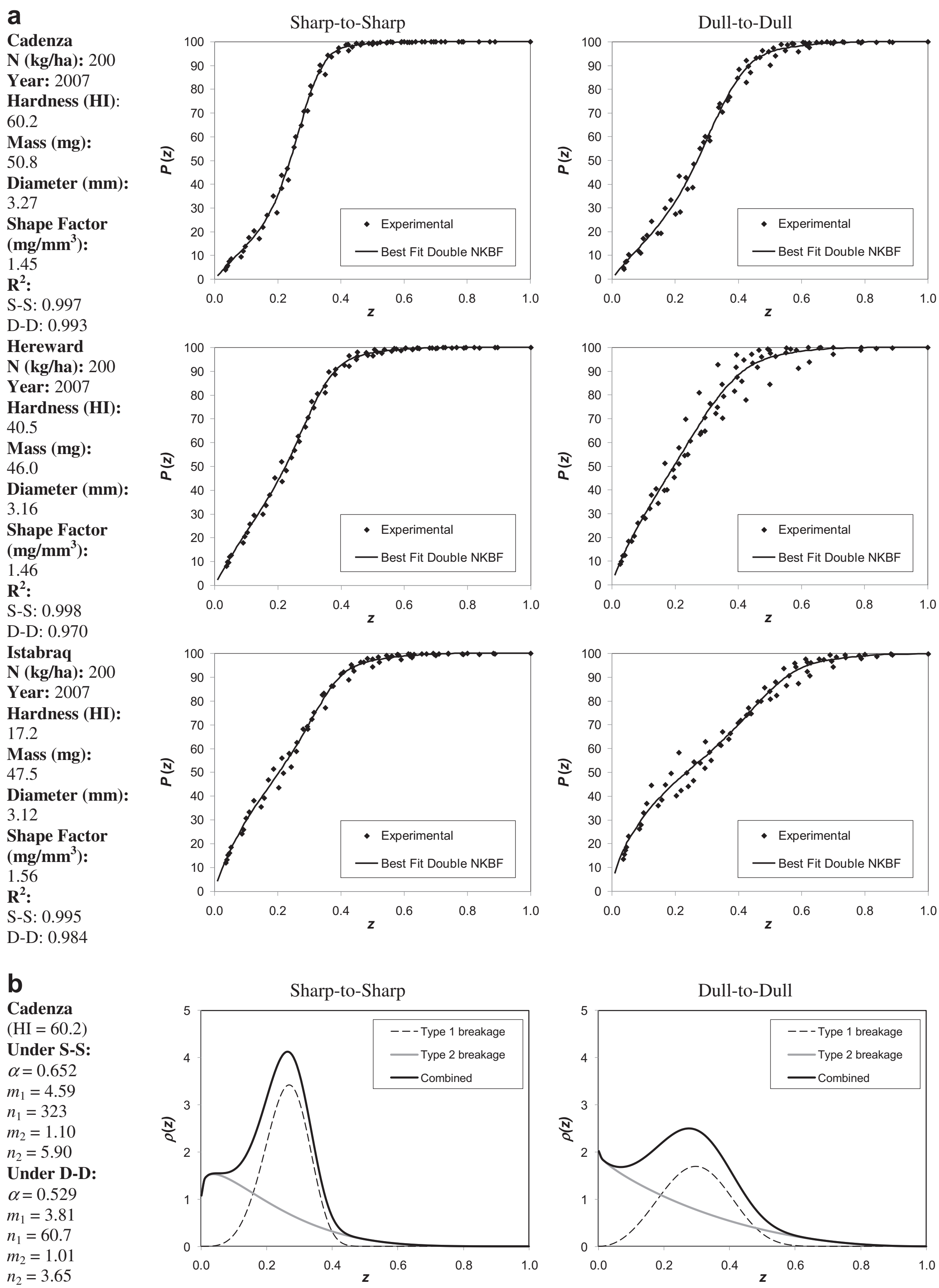

Fig. 2. (a) Collapsed data resulting from milling wheats at five roll gaps, and the best fit Double NKBF; and (b) Best fit Double NKBF, in its non-cumulative form and illustrating Type 1 and Type 2 breakage, for three representative wheats under Sharp-to-Sharp and Dull-to-Dull milling.

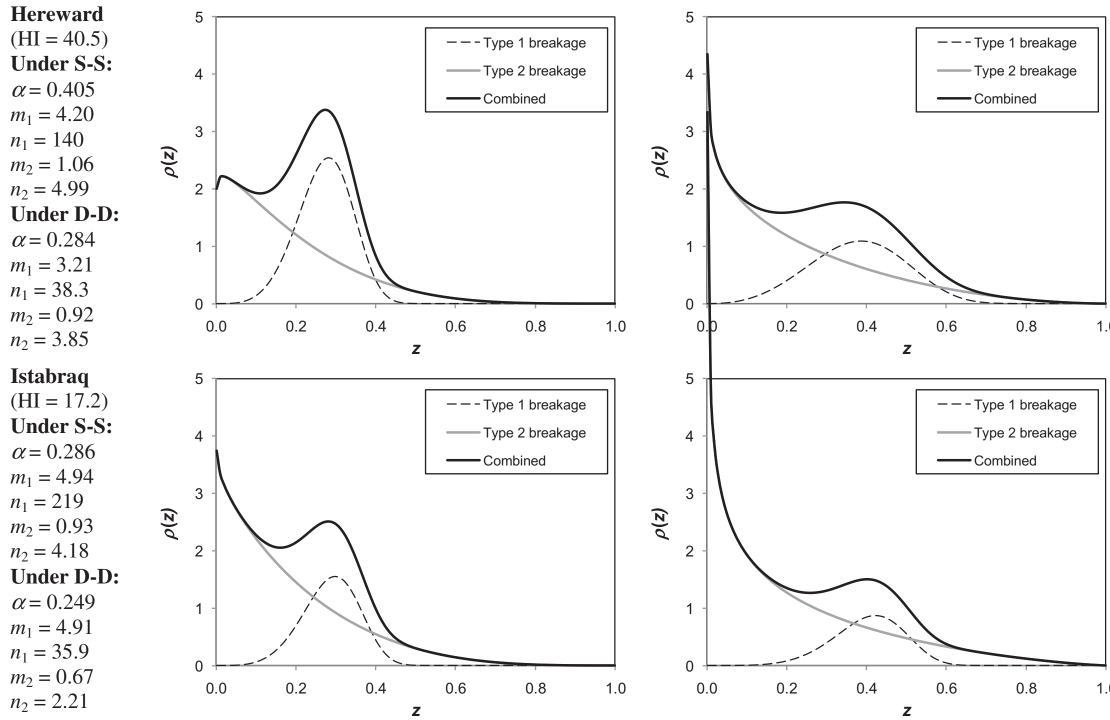

Fig. 2. (*continued*).

their non-cumulative form for each of the three wheats, and the combined non-cumulative psd. These curves were generated from the best fit values of α, m_1, n_1, m_2 and n_2, for each wheat under each disposition. Clearly, D–D milling gives a flatter, broader psd, with relatively more small and large particles than S–S milling, and hence fewer in the mid-sized range. Similarly, the softer Istabraq breaks to give greater proportions of both small and large particles, while the harder Cadenza results in a greater concentration of mid-sized particles. These observations are consistent with previous work (Campbell et al., 2007; Fang and Campbell, 2003a) and give a fuller picture, as they now cover the full particle size range.

Fig. 2(b) reveals the different features of the two parts of the DNKBF, which we have called for convenience Type 1 and Type 2 breakage. Type 1 breakage, it now becomes apparent, describes a narrow peak of mid-range particles, generated by values of m_1 typically around 5, and of n_1 typically >100. Type 2 breakage is described by values of m_2 of around unity and of n_2 of around 2–6 and appears to describe principally the small particles, but with a long tail that extends to the very large particles. (As m_2 crosses from <1 to >1, a small peak occurs in the curve described by Type 2 breakage; this may not be meaningful regarding the actual psd of the broken particles, but it illustrates the mathematical effect of the m parameter in the NKBF.).

One must be cautious in assigning physical meanings to a convenient mathematical description; the DNKBF is a convenient function with sufficient flexibility to describe wiggly particle size distributions, but that does not give it inherent meaning based on fundamental physical relationships. Nevertheless, it is reasonable to recall that roller milling of wheat is employed because it tends to break wheat kernels such that the bran remains in large particles and the endosperm shatters into smaller particles. The distinct patterns of Type 1 and Type 2 breakage thus suggest that Type 1 breakage is perhaps principally associated with breakage of the bran material into large particles, while Type 2 breakage is principally associated with breakage of endosperm into small particles. However, the Type 2 breakage also appears to describe the very large particles. This may be an artefact of the constraints of fitting the data, such that this small proportion of large particles happens to be more conveniently described via the Type 2 curve, with the values of its parameters principally influenced by the large amount of small endosperm material. However, it also suggests an alternative interpretation of Type 1 and Type 2 breakage, not based on bran and endosperm, but based on the two principal breakage mechanisms, crushing and shearing (to which bran and endosperm respond differently). In the absence of experiments aimed at illuminating the physical mechanisms underlying Type 1 and Type 2 breakage, it is premature to speculate; further work will investigate the interpretation of these breakage patterns directly.

Returning to Fig. 1(b), we observe that Type 2 breakage dominates for D–D and for soft wheats; this is the breakage mechanism that generates many small particles and also accounts for the very large particles. Type 1 breakage, by contrast, generates a narrow distribution of relatively large daughter particles, and is prevalent under S–S milling and for harder wheats. It is known that soft wheats tend to shatter easily into numerous small endosperm particles, while leaving the bran material relatively intact as large particles, while hard wheats transmit the stresses throughout the kernel, such that the endosperm resists shattering and breaks together with the bran (Pomeranz and Williams, 1990). Thus Type 1 breakage becomes increasingly dominant as hardness increases, as is evident in Fig. 1(b).

In addition to giving potentially useful mechanistic insights into breakage, the power of the DNKBF is to allow prediction of breakage based solely on SKCS parameters, principally hardness. To this end, it is necessary to establish the relationships between the DNKBF parameters and SCKS hardness. Fig. 1(c)–(f) shows the variations in m_1, n_1, m_2 and n_2 with SCKS hardness, under both dispositions. Under S–S, m_1 hovers consistently around a value of about 4.5, while n_1 similarly shows little relation to hardness, although with wide variation. This variability, and the lack of variation with hardness, arises because Type 2 breakage dominates, such that the parameters m_1 and n_1 describe relatively little of the variation and are thus not fitted very accurately. Nevertheless, under D–D there are more evident effects of hardness on m_1 and n_1, requiring quadratic equations for their description. Considering m_2 and n_2, in all cases there appears to be a strong positive linear correlation with hardness. For m and $n > 1$, a peaked curve results; an increase in m tends to move the peak to the right, while an increase in n tends to move it to the left. Simultaneous increases in these two parameters tend to move the Type 2 breakage curve more to the right, reducing the proportion of small particles. Thus, harder wheats give larger Type 2 particles, and more Type 1 breakage which also favours larger particles; together these imply larger particles and a narrower range of particle sizes for hard wheats.

Fig. 1 shows the equations relating SKCS hardness to the various parameters of the DNKBF. These relationships allow prediction of the breakage of any wheat based solely on SKCS hardness and diameter. These equations are able to predict the entire psd over the range 0–4000 μm, for wheat of any size and hardness at any roll gap, using a total of 11 coefficients under S–S and 13 under D–D. This compares favourably with the 24 coefficients required by Campbell et al. (2007) to predict just the 0–2000 μm range. Using these equations, the mean coefficient of determination, R^2, between the predicted cumulative psd and the collapsed experimental data was 0.994 for S–S and 0.980 for D–D.

However, Fig. 1 shows considerable scatter in the datapoints, implying that SKCS hardness cannot completely account for the variation in breakage during roller milling, and there were some wheats for which the predictions were poor. As with the work of Campbell et al. (2007), it was desired to investigate, using this larger dataset, whether the fourth SKCS parameter, kernel mass, could explain some of the residual variation. A long, thin kernel should have a greater mass than a short kernel of the same SKCS diameter, for a constant density; thus the ratio of SKCS mass to D^3 should give an indication of kernel shape, and this might be expected to relate to breakage.

Following the approach of Campbell et al. (2007), a residual analysis was performed to relate the residual variation to SKCS mass, M, and to the shape factor, M/D^3. The residual curve as a function of z was calculated by subtracting the value of $P(z)$ predicted by the DNKBF (given by Eq. (5) and the equations in Fig. 1) from the value resulting from the best fit of Eq. (5) to the collapsed data. It was rationalised that the DNKBF would tend to overpredict or underpredict, such that the residual curve would tend to be predominantly positive or negative. The area under the residual curve was therefore calculated by numerical integration. A positive value of the residual implies overprediction, i.e. the wheat breaks to give smaller particles than predicted. This residual area was then plotted against SKCS mass and shape factor, to identify whether these were responsible for observed variations in breakage not explained by SKCS hardness.

Fig. 3 shows the correlation between residuals calculated for S–S and for D–D. These are strongly correlated; a given wheat tends to be consistently overpredicted or underpredicted under both dispositions, giving confidence that these residuals are meaningful. From the slope of the regression line, the residual under D–D was on average about 65% larger than the residual under S–S. The units of this residual area are %; its value represents the average departure of the predicted cumulative particle size distribution from the best fit distribution. From Fig. 3, the average deviation was in most cases less than 2 percentage points under S–S, and less than 5 percentage points under D–D.

Fig. 4 illustrates several sets of data with the corresponding best fit DNKBF and the DNKBF predicted from SKCS hardness. The curves

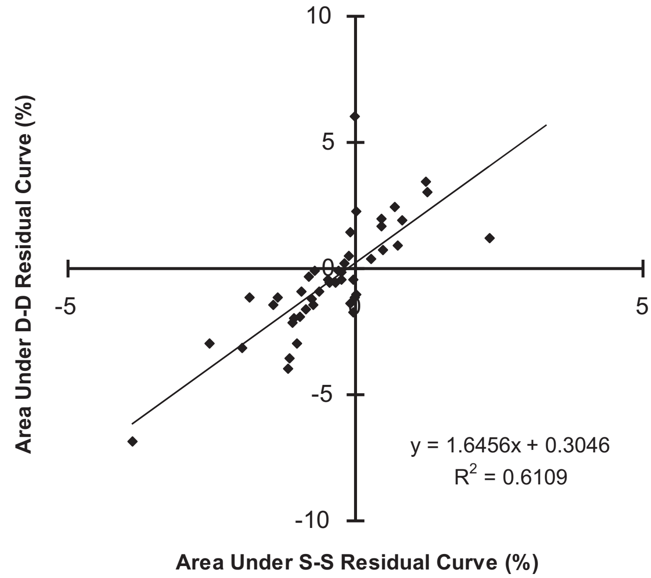

Fig. 3. Correlation between residuals under Sharp-to-Sharp and Dull-to-Dull milling.

illustrate an overpredicted curve with a positive residual and an underpredicted curve with a negative residual, under both dispositions. These examples have been selected to allow the fitted and predicted curves to be clearly discriminated; in most cases the agreement was much closer than shown here.

Fig. 5(a) shows the plot of residuals *versus* shape factor for both S–S and D–D. Disappointingly, there is little correlation and insignificant correlation coefficients. Differences in particle size distributions on breakage do not appear to relate easily to shape as indicated by SKCS mass and diameter. Plotting residuals against kernel length:width ratio raised the correlation coefficient to about 0.2 under both dispositions (results not shown). However, Fig. 5(b) shows the plots of residuals *versus* SKCS mass. In this case there are significant positive correlations; heavier kernels tend to be overpredicted, and lighter kernels underpredicted. The correlation is weaker under S–S; this is because the predictions for S–S based on hardness are already excellent, with little scope for improvement. For D–D, mass explains 25% of the residual variation (rising to 33% if the largest outlier, resulting from the 2007 200 kg/ha Hereward sample, is removed).

Although the correlation with shape factor is insignificant, its negative value makes sense in physical terms; the negative slope implies that elongated kernels are underpredicted, i.e. they break to give on average larger particles than predicted from their hardness. Less elongated, more spherical kernels are overpredicted; they break into smaller particles on average than expected from their hardness. Elongated kernels have relatively larger surface areas than more spherical kernels, and hence a higher proportion of bran (ignoring crease and bran thickness effects, to a first approximation, kernels with a larger surface area will have a higher bran content.) It is also known that bran tends to break into larger particles. Thus, it is perhaps not surprising to find that the extra bran content of elongated kernels gives a greater proportion of large particles and hence larger average particle sizes than expected.

In addition to this physical explanation that is consistent with the negative correlation, further studies by Mazlan (2010) and Coate (2011), using different wheat sets under D–D milling, also gave slightly negative correlations. The current availability of four datasets (three under D–D and one under S–S milling) consistently showing this slight negative correlation, together with the physical

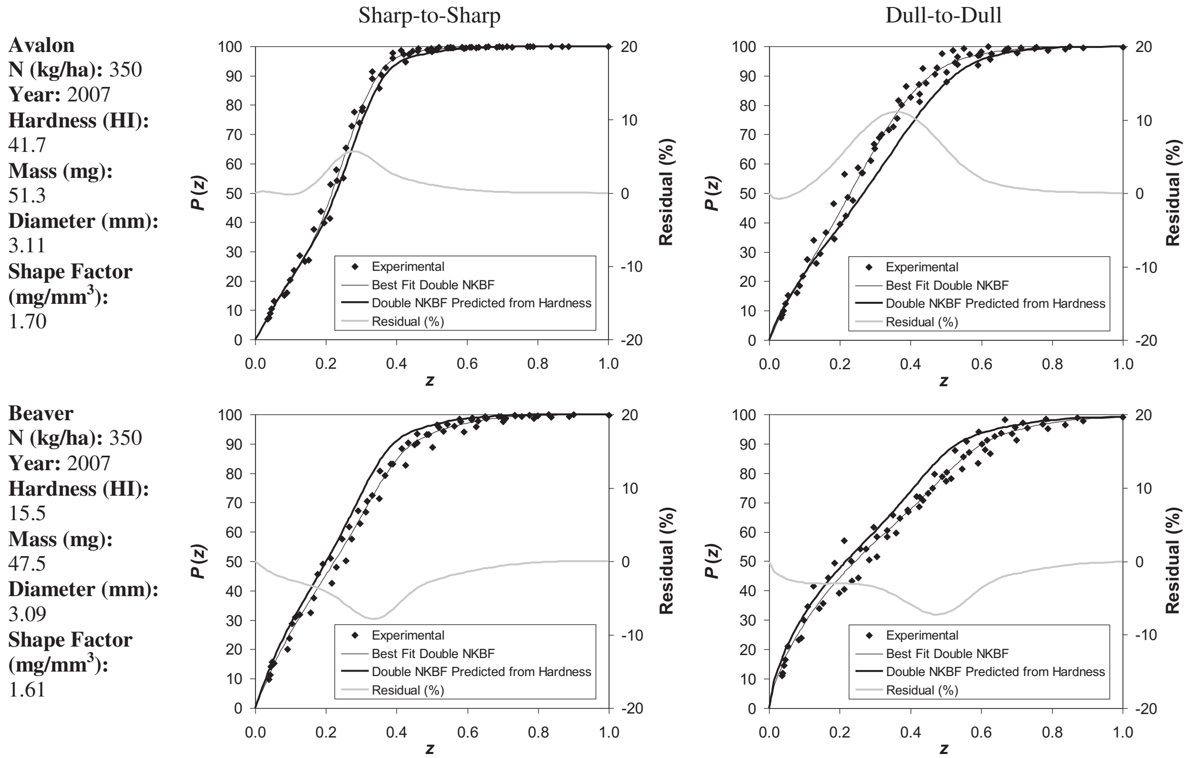

Fig. 4. Examples of best fit Double NKBF curves and curves predicted from hardness, illustrating residual calculations, for an overpredicted wheat (Avalon) and an underpredicted wheat (Beaver) under Sharp-to-Sharp and Dull-to-Dull milling.

explanation discussed above, combines to give quite strong evidence that kernel shape affects breakage, with elongated kernels giving relatively larger particles, compared with more spherical kernels.

The results offer further encouragement that wheat hardness, as measured by the SKCS, is meaningful in relation to actual breakage during roller milling. As noted by Campbell et al. (2007), this is a surprising but convenient finding – surprising, because the breakage mechanism in the SKCS is very different from the breakage action during First Break roller milling, but convenient, because it allows prediction of milling directly from SKCS hardness. But why does shape show little relation to residual, whereas mass does? It must be remembered that SKCS hardness is an arbitrary number, nominally ranging from 0 to 100, calculated from the fundamental data using an undisclosed algorithm (Osborne and Anderssen, 2003). The observation that kernel shape appears to have little effect on breakage implies that variation in grain shape is interpreted by the SKCS as hardness, which then correctly predicts the effects of this variation on breakage. Consequently, shape is already accounted for when relating hardness to breakage and little further improvement in prediction is possible. However, the observation that the residual variation appears to be related to kernel mass is probably best interpreted as indicating that the SKCS hardness algorithm does not take account of mass as appropriately as it should. Slightly modifying the SKCS hardness algorithm to reflect the mass effects reported here may yield a hardness index that more accurately represents breakage during roller milling.

The finding that SKCS hardness predicts most of the breakage during roller milling, such that there is little variation left to be explained by shape, and the suggestion that this is because the SKCS interprets shape variation as hardness, is convenient from a practical perspective, because it allows prediction of breakage based solely on SKCS size and hardness, but it is frustrating from a scientific perspective, because it hinders the effects of kernel shape on breakage from being independently distinguished. It also raises an interesting observation about the meaning of 'hardness' as applied to wheat, that cereal scientists use the term 'hardness' to mean two different things. Wheat hardness refers to the mechanical properties of the endosperm and the molecular and genetic origins of these; wheats are genetically determined to be hard or soft largely by the presence of genes, encoding two puroindoline proteins, at the *Hardness* (*Ha*) locus, which confer softness (Greenwell and Schofield, 1986; Pomeranz and Williams, 1990; Simmonds et al., 1973; Turnbull and Rahman, 2002). But wheat hardness also refers to "the way the wheat breaks during milling", which depends on the endosperm mechanical properties but also on the bran properties and the kernel morphology. These two views of hardness are correlated, clearly, but are not the same thing. The SKCS measures the force profile during crushing; it measures "the way the kernel breaks". This measurement does not solely reflect the endosperm mechanical properties but also the kernel shape, crease morphology and bran mechanical properties. Thus, although SKCS hardness is a good indicator of wheat breakage, it may not be a precise indicator of the endosperm hardness. For most practical purposes the distinction is likely to be unimportant, but it may be significant when the aim is to distinguish between effects of other factors such as shape on breakage, as in the current work, or to understand clearly the nature or origins of endosperm hardness.

It is therefore likely that kernel shape influences breakage, but the SKCS obscures this by interpreting these effects in the reported hardness index. If a measure of hardness were used that related more purely to endosperm hardness, uninfluenced by bran and by shape effects, then the above analyses could be repeated, correlating NKBF parameters with this measure of true endosperm hardness rather than SKCS hardness. In this case, the predictions might be expected to be less accurate than those obtained from

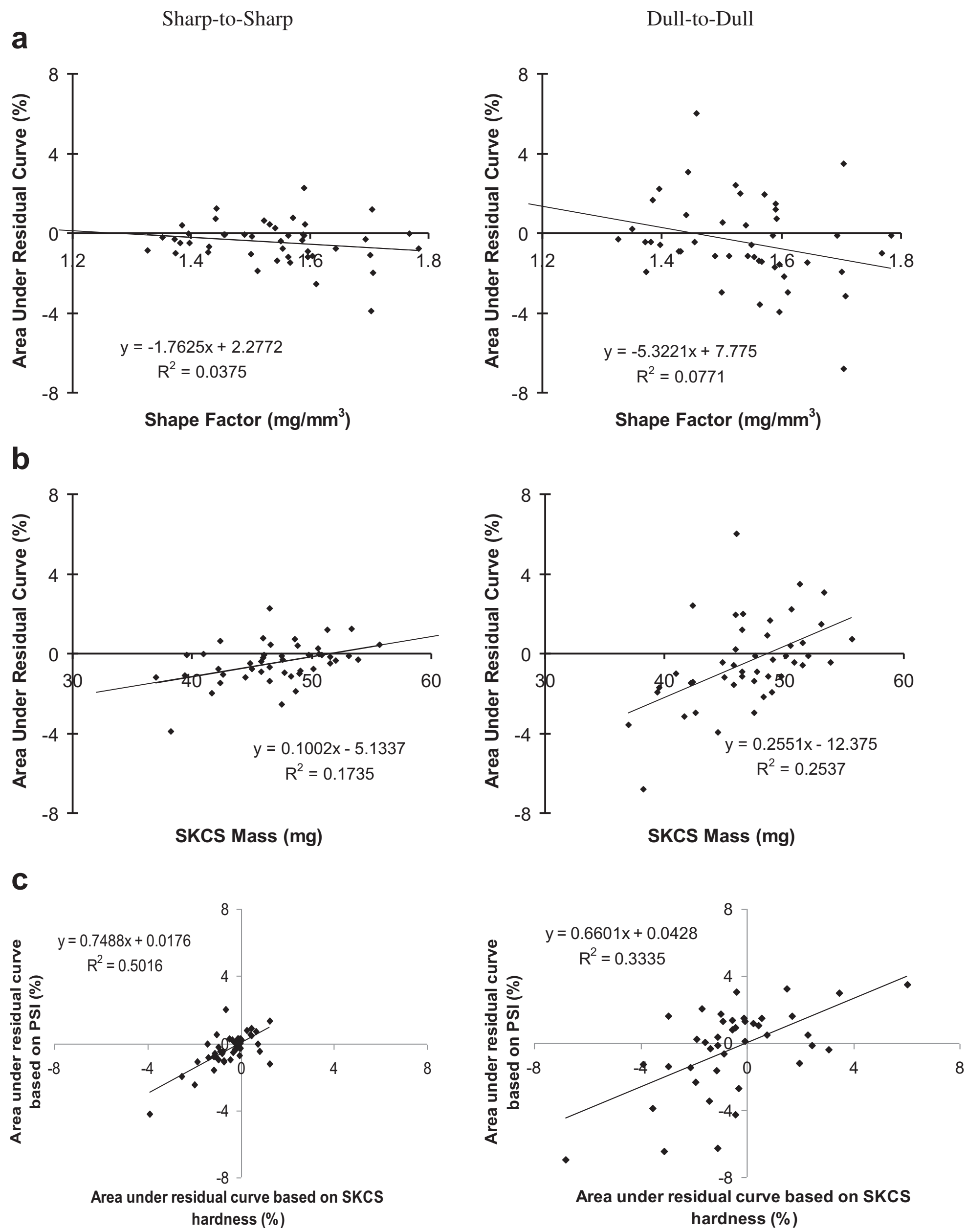

Fig. 5. Residual variation *versus* (a) shape factor; and (b) SKCS mass for Sharp-to-Sharp and Dull-to-Dull milling; and (c) Residuals based on Particle Size Index *versus* Residuals based on SKCS hardness.

SKCS hardness, leading to larger residuals, and allowing shape effects on these residuals to emerge more clearly.

The above hypothesis was tested by reanalysing the data using Particle Size Index (PSI) rather than SKCS hardness, on the basis that PSI is a more fundamental measure of endosperm hardness (and is used as such to calibrate SKCS hardness). In fact, PSI gave even better predictions and slightly lower residuals. Fig. 5(c) shows the residuals resulting from using PSI *versus* those resulting from using SKCS hardness, under S–S and D–D milling. As before, predictions were better for S–S than for D–D, as indicated by the smaller values of the residual areas. From the slopes of the regression lines, the PSI-based residuals under S–S were on average only 75% of the corresponding SKCS hardness-based residuals, while under D–D the ratio was 66%. Thus, predictions based on regressions of DNKBF parameters against PSI were slightly more accurate than those based on SKCS hardness.

The hypothesis was that, because PSI is quantified in terms of the size distribution of flour particles released on milling, it was a ‘purer’ indication of endosperm hardness that would be unaffected by bran or kernel shape. The better predictions given by PSI suggest this hypothesis may not be valid. From our general understanding of milling, it is known that small particles of endosperm are scraped off large bran particles, due to the differential action of the roller mill. Thus it may be that the milling process used to generate the small particles measured in the PSI test does so by scraping from larger bran particles, and that PSI measurements of hardness are not therefore independent of bran characteristics. Furthermore, the more extensive milling process used in the PSI test, relative to the breakage occurring in the SKCS, means the former is arguably closer in nature to roller milling, hence its ability to give better predictions of breakage during roller milling.

5. Conclusions

Breakage of wheat during roller milling can be described by the DNKBF, which appears to reveal particle size distributions resulting from two breakage mechanisms, one of which results in numerous small endosperm particles and a tail of very large bran particles, while the other results in a narrower distribution of mid-sized particles. The former dominates for soft wheats and under Dull-to-Dull milling, while the latter becomes more prominent for harder wheats and under Sharp-to-Sharp milling. The parameters of the DNKBF were correlated with wheat hardness, allowing prediction of the breakage of wheat at any roll gap based on the hardness and diameter values reported by the Single Kernel Characterisation System. A residual analysis suggested that more elongated kernels tend to break to give on average larger particles than predicted from their hardness.

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