Discrete Element Method as an Approach to Model the Wheat Milling Process

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Abstract

It is a well-known phenomenon that break-release, particle size, and size distribution of wheat milling are functions of machine operational parameters and grain properties. Due to the non-uniform characteristics and properties of wheat kernels, the kernel physical and mechanical properties affect the size reduction process. This research was the first to test the functionality of the discrete element method (DEM) to simulate the 1st break wheat roller milling process. DEM models of 1st break wheat milling were developed by incorporating the bonded particle model along with the spherical-shaped and kernel-shaped particle models. The models simulated hard red winter (HRW) wheat milling at 12%, 14%, and 16% moisture content and was validated using lab scale milling trials. The spherical-shaped approach simulated the size reduction of a

spherical cluster of mono-sized particles with uniform bond strength throughout the kernel. At 16% moisture content, this spherical-shaped kernel model resulted in an average particle size of 438 μm with a deviation of prediction of 177%. The prediction error was reduced to 144% with a mean PSD of 372 μm by modifying the shear modulus and coefficient of restitution values. With the kernel-shaped model, a bonded cluster resembling a wheat kernel in shape and size was used with a random distribution of particle bond strengths in the kernel. Even though the model predicted a 1st break particle size of 413 μm , which had a deviation of 139% from the lab scale milling results, the model satisfactorily predicted the variation in particle size distribution from 1st break milling with moisture content.

1. Introduction

Wheat milling is a gradual size reduction process involving separation of the endosperm from the bran layers and germ, and subsequently reducing the size of the endosperm to flour. This is achieved by a series of size reduction operations that include break and reduction roll systems, sifters, and purifiers [1]. Different milling systems are used for size reduction of wheat, but, studies have indicated that roller milling is more efficient than hammer milling or stone milling [2]. The purpose of any commercial flour mill would be to meet the needs of their customers by providing the highest quality flour at maximum flour extraction rate thereby enabling maximum profits. However, the extraction rate and quality of flour are directly dependent on the efficiency of separation of the endosperm from the bran layers. In addition, the size reduction achieved at the first break roll system regulates the flow of mill streams through the other milling operations. Detailed explanation of wheat milling can be found elsewhere [3, 4].

At first break, wheat kernel physical, mechanical properties, and machine operational variables influence the size reduction and separation of the endosperm. The grain properties include kernel size, hardness, moisture content, and bulk density; and machine operational parameters include roll gap, feed rate, roll disposition, and roll speed differential. The effect and significance of these variables on the milling process have been studied using different modeling techniques. Some of the reported techniques include surface regression response modeling [5], neural network modeling [6], linear regression modeling [7], and modeling based on breakage behavior [3]. Though these modeling techniques predicted the size of ground wheat, but, these statistical models were based on existing data. The major concern with these models was they did not account for the non-uniform physical and mechanical characteristics of wheat kernels.

The discrete element method (DEM) is a numerical modeling technique that can solve problems in engineering that display discontinuous behavior. DEM takes into account physical and mechanical properties of the particles as input parameters to predict future motion or deformation. Over the past decade, extensive work has been conducted on using DEM to predict granular food material production/handling processes [8, 9]. DEM predicts the flow of individual particles and their collisions, contacts, and interactions with other particles and their surrounding environment [10]. To predict the particle-particle interaction, DEM makes use of various contact models and force-velocity-displacement laws [11]. The simplest mechanical system is a linear spring-dashpot model proposed by Cundall and Strack [12] where the spring accounts for the elastic deformation and the dashpot accounts for the viscous dissipation. One of the common variations of the linear spring-dashpot model is the more complex and accurate, Hertz-Mindlin and Deresiewicz model [11, 13].

Uniform breakage during size reduction is a challenge across the solids processing industry. Efforts had been made to study the breakage phenomenon using simple breakage models in DEM. Cleary [14] discussed the applications of DEM in modeling cement milling, size reduction in a SAG mill and tumbling mills [15]. Majority of these studies focused on studying the breakage and flow of particles inside the mill rather than the bonding of particles. In 2004, Potyondy and Cundall [16] developed a bonded-particle model (BPM) to predict rock breakage. Their pioneering work led to application of DEM for studying particle breakage, comminution, and size reduction. Metzger and Glasser [17] incorporated the BPM in the DEM framework to study the breakage of agglomerates in ball mill and successfully determined the parameters that affected breakage. With their work they were also able to demonstrate the applicability of DEM in analyzing various aspects of particle breakage in ball mills. Quist [13] also used the BPM to predict rock breakage in a cone crusher. Both of these studies extensively used BPM in DEM to create non-spherical shaped agglomerates. A comprehensive review of literature on application of DEM in comminution and size reduction has been provided elsewhere [18]. Though many studies have predicted the size reduction of rocks and pharmaceutical solids, there is lack of DEM models to predict the milling of cereal grains. Non-uniform physical characteristics (size, shape, density), chemical composition (bonding strength between different components), and mechanical properties (fracture strength, compaction) make it challenging to develop a DEM model. This study is a first attempt to predict the size reduction of wheat using a numerical approach. The objectives of this research are: i) to develop a DEM model to predict the wheat milling process using the BPM approach and ii) to validate the model with laboratory scale and industrial scale milling experiments. Because wheat milling involves

progressive size reduction with multiple grinding, this study was limited to predicting the wheat kernel breakage at the first stage of milling (1st break).

2. Materials and Methods

2.1. Model set-up

The Hertz-Mindlin with bonding contact model was used in this study. This model enables calculation of forces acting on a particle due to its interactions with other particles and surfaces based on the Hertz-Mindlin with no slip contact model. BPM was used to introduce bonds between the particles within a wheat kernel. The bonds are defined with specific parameters of the BPM, such as the bond stress and stiffness values. The bond between each particle is modeled as a set of elastic springs distributed over a circular cross section that transfers the translational and rotational motion experienced by one particle to the other particle it is bonded to [18]. The 1st break wheat milling process was simulated with a spherical-shaped and a kernel-shaped model of the wheat kernel. The DEM simulations were carried out using EDEM 2.6 (DEM Solutions Ltd., Edinburgh, UK) software installed on an Intel Core 2 Duo processor with 4 GB RAM and 64-bit Windows 7 professional operating system.

2.2. Creating geometry

The 1st break roll mill geometry was created in AutoCAD 2013 (Autodesk Inc., California, USA) and the specifications used to create the roll stand are given in Table 1. The geometry was then imported into EDEM as an *.iges* extension format input. The rolls (Fig. 1) were fixed to rotate around an axis at a fixed speed maintaining a speed differential of 2.5:1 with a dull-to-dull grinding action. This creation of geometry with actual mill parameters enabled simulating a laboratory scale milling process.

2.3. Particle creation

After importing the geometry into EDEM, particles were created and assigned with physical and mechanical properties of the kernel or wheat mill stream being modeled. The 1st break stream particles were assumed to be of spherical in shape (Fig. 2 B, D). Here onwards, the wheat kernel and 1st break particles will be referred to as whole particles and fraction, respectively. After creation, the physical and mechanical parameter values were defined for these particles. Wheat kernels consist of endosperm, bran, and germ. For simulation purposes, the particle cluster within a wheat kernel was created by bonding spherical particles representing different components of a wheat kernel. The cluster replaces the whole kernel (Fig. 2) using the particle replacement factory. This cluster of fraction particles bonded together then represented the wheat kernel. Detailed explanation on creating custom factory with bonded cluster and particle replacement factory can be found elsewhere [13].

In this study, properties of hard red winter (HRW) wheat kernels were used as input parameters. The measured values of whole particles and fraction [1] for size, size distribution, density, shear modulus, coefficient of static and rolling friction, and coefficient of restitution were used as input parameters. Published literature values of Poisson's ratio and shear modulus values were used [19, 20, 21]. All input parameters are listed in Table 2. Because wheat kernel milling moisture content ranges from 12 to 16% (wet basis), input parameters at three moisture content levels were used in this study. This range was also used to observe the effect of moisture content on model prediction.

2.3.1. Sphere-shaped approach

In this approach, the wheat kernel was assumed to be a sphere. Then the spherical shape was created by filling with spherical break stream particles as shown in Fig. 2 A and B. To

simulate the milling process using this approach, the following assumptions were made, i) the bran and flour particles are uniform in size and shape; ii) the wheat kernel is comprised of the cluster of bonded flour and bran particles; iii) bond strength is uniform within the kernel.

2.3.2. Kernel-shaped approach

For the kernel-shaped approach, the overall kernel shape was based on four overlapping spheres layered together and filled with smaller sized particles (bonded together) as shown in the Fig. 2 C and D to approximate the true shape of a wheat kernel. The bond strength in the multi-layered kernel was distributed (Table 3) to replicate the differences in the characteristics of endosperm, bran layer, and germ.

2.3.3. Particle bonding and breakage

To introduce bonds between the particles, the Hertz-Mindlin with bonding contact model was used based on the bonded particle model (BPM) approach developed by Potyondy and Cundall [16]. This model incorporates the working principle of both Hertz-Mindlin with no slip contact model for particle interaction and BPM for bond formation and breakage. Bond formation between particles primarily depends on the bond start time, and the bond radius. The bond start time is the time at which the model creates bonds between the particles in contact. At the bond start time, the whole particles were replaced by the cluster of fraction particles using the particle replacement factory. In the immediate next time step, bonding was introduced between the particles of the cluster to retain the spherical shape of the cluster. At this particular time, a parallel bond is formed between all the particles in contact with other particles provided the extent of this overlap falls within the bond radius. The overlap between the particles is an indication of the deformation taking place due to particle-particle interaction. Fig. 3 represents the schematics involving two particle bonding and the resultant force and torque. The strength of

this parallel bond formed between two particles depends on the shear stress and the stiffness values (Table 3) calculated using the following equations:

$$\Delta \bar{F}^n = \bar{k}^n A \Delta U^n \quad (1)$$

$$\Delta \bar{F}^s = -\bar{k}^s A \Delta U^s \quad (2)$$

$$\Delta \bar{M}^n = -\bar{k}^s J \Delta \theta^n \quad (3)$$

$$\Delta \bar{M}^s = -\bar{k}^n I \Delta \theta^s \quad (4)$$

Similarly, the maximum force the bond withstands is predetermined using the following equations. A force exceeding this pre-set critical stress values results in the breakage of the bonds.

$$\bar{\sigma}_{max} = \frac{-\bar{F}^n}{A} + \frac{|\bar{M}^s| \bar{R}}{I} < \bar{\sigma}_c \quad (5)$$

$$\bar{\tau}_{max} = \frac{|\bar{F}^s|}{A} + \frac{|\bar{M}^n| \bar{R}}{J} < \bar{\tau}_c \quad (6)$$

where, $\bar{F}^n$, $\bar{F}^s$, $\bar{M}^n$, $\bar{M}^s$ denote the axial – and shear – directed force and moments respectively; U^n , U^s , θ^n , θ^s denote the relative displacement – and rotation component in the axial and shear directions; A , I , J are the area, moment of inertia and the polar moment of inertia of the parallel bond; $\bar{\sigma}_{max}$, $\bar{\sigma}_c$, $\bar{\tau}_{max}$, $\bar{\tau}_c$ denote the maximum and critical tensile stress and shear stress cutoff values the bond can withstand; and $\bar{R}$ denotes the parallel bond radius. If any of the critical values is exceeded, the bond breaks.

2.4. Model functionality

On completion of the milling simulation, the mass and volume data of the particles obtained from the model at each time step was exported into a Microsoft Excel spreadsheet

(Microsoft Corporation, Washington, USA). This data was used to calculate the mean particle size and size distribution.

To determine the functionality of the spherical-shaped and kernel-shaped modeling approaches, validation experiments were conducted using the Ross tabletop experimental roller mill (Ross, Oklahoma, USA) at Kansas State University. Moisture content of wheat kernels were adjusted to 12%, 14%, and 16% (wet basis) by adding the required amount of water based on initial moisture content and dry matter content [22]. The moisture was added to the sample in a wheat tempering equipment (tumbler) and the sample was mixed for [60 min] and allowed to equilibrate for 12 hours.

The roll (1st break) was adjusted to a speed differential of 2.5:1. The roll gap was set at 6.35 mm. Three milling trials using 1000 g wheat per trial at each moisture level were performed. The size reduction at each trial was determined by calculating the percent ground wheat passing through the 1041 μm (US 20SSBC) sieve opening when sifted for 2 min. The sifting was done through a Great Western Lab Sifter (Great Western Co., Kansas, USA) with a sieve stack of 20SSBC (1041 μm), 50GG (375 μm), 70GG (240 μm), 10XX (132 μm) and pan [23]. The particle size distribution of the milled samples was determined using ASABE Standard S319.4 [24], by sifting the material for 15 min in the following stack of sieves: 20 SSBC (1041 μm), 24SSBC (869 μm), 10XX (132 μm), and pan.

The mean relative deviation of the particle size and size distribution obtained from the model and the milling trials was determined using the following formula:

$$P = \frac{100}{N} \times \sum \frac{|Y - Y_p|}{Y} \quad (7)$$

where Y is the experimental value; Y_p is the predicted value; and N is the number of observations (number of sieve openings) that were used to calculate the mean geometric particle size.

2.5. Sensitivity analysis

A sensitivity analysis was conducted for the spherical-shaped model by varying the shear modulus and coefficient of restitution property values. Because most of the other parameters were measured, sensitivity analysis was conducted only for these two parameters that were adapted from literature. A wide range of values have been published for the elasticity modulus of wheat kernel [19, 25, 26] and wheat kernel endosperm [27, 27, 29, 30]. Using the elasticity modulus, the shear modulus for wheat and endosperm was calculated using the relationship given by Boac et al [31]. The calculated shear modulus values ranged from 0.53 to 76.5 MPa.

Due to the non-availability of shear modulus values for the 1st break stream, the same value range used for wheat and endosperm was used for the sensitivity analysis. The properties listed in Table 2 were used to calibrate the model. Sensitivity analysis was performed in two steps. First, the milling process was simulated by adjusting the shear modulus values at 1, 10, 20, 30, 40, 50, 60, 65, 70, and 76.5 MPa. The resulting mean geometric particle size and size distribution obtained from each of these simulations were compared with the lab-scale milling results of HRW wheat at 16% moisture content (wet basis) until obtaining a lowest mean relative deviation. In the next step, the coefficient of restitution was adjusted by keeping the shear modulus constant. The coefficient of restitution was varied as 0.30, 0.25, 0.2, 0.15, 0.1, 0.05, and 0.01 until least mean relative deviation was obtained.

3. Results and Discussion

For a simulation run time of 1s, it took an average of 72.4 hours of computing time for the sphere-shaped model and 200.6 hours for the kernel-shaped model to complete the milling process. The particle cluster broke, simulating milling, when the kernels passed through the rolls due to the breakage of the bonds between the particles. During milling, with the roll gap smaller than the size of a wheat kernel and due to the roll speed differential, compressive and shear forces acted upon the kernels. When these forces exceeded the critical stress or stiffness value, the bond between the particles started breaking and releasing the particles from the cluster. Figure 4 shows the breakage of bonded cluster and the bonds between particles as it passes through the break rolls in progressive time steps. Based on the input parameters used, the minimum force required to break the bond was calculated from the bond strength and contact radius values using the relation between the stress and force application. In the kernel-shaped model, a minimum force of 6.25 N is required to break the particle bonds.

3.1. Sphere-shaped approach

In this simulation of the wheat milling process, it was assumed that the particle cluster would break into either individual particles it is made up of or into smaller clusters. The size and size distribution of the milled particles were plotted as a cumulative distribution of the percent mass of sample collected at three sieves i.e. 20SSBC (1041 μm), 24SSBC (869 μm), 10XX (132 μm), and the pan (Fig. 5). The particle size distribution was then used to calculate the average particle size and the deviation in prediction (Table 4).

The model predicted an increase in the particle size of 1st break stream with increase in moisture content of wheat from 12 to 16%. This was validated by lab scale milling trials, which also displayed a similar trend. At all the moisture levels, it was found that there was a large

deviation in predictions of the model from the lab scale trial results. On breaking down the model predictions obtained from 1st break simulations, it was found that there were no particles larger than 1041 μm or smaller than 132 μm . All particles were within $>132 - <1041\mu\text{m}$ range. Conversely, the lab scale milling resulted in approximately 69% of particles over 1041 μm and about 4% of break flour passing through 132 μm sieve opening with a break release of 31% (Break release is the amount of flour collected at a milling step). Due to the wider particle size distribution obtained during lab scale milling, a high mean relative deviation from the model results was observed. Metger and Glasser [18] in a study investigating the breakage of agglomerates during impact reported that the use of a constant bond strength almost always resulted in breakage of the agglomerate into single individual particles and not into fragments of intermediate size. Similar claims were made by Thornton et al. [33] who established the Johnson-Kendall-Roberts (JKR) theory to study fracture of agglomerates.

The high mean relative deviation could be attributed to two causes. First, in the model, spherical agglomerates made up of uniformly sized spherical particles were used to represent the wheat kernel. Secondly, uniform bond strength was used to bond the particle cluster. During simulation of size reduction, the wheat kernel agglomerate breaks into individual spheres or agglomerates representing flour, bran, and endosperm. However, during the wheat milling process, the kernel does not break into chunks of uniformly sized particles. Instead, due to the compression and shear forces, the kernels break into bran, endosperm, and some amount of flour resulting in a wide size distribution. Furthermore, the shapes of particles are not spherical. Due to the difference in shape and the size of the particles from the model and the milling trial, this variation was observed. Due to the uniform bond strength, size reduction resulted in majority of the clusters breaking up into individual particles with only a minimum percentage of clusters. In

addition, the model predictions did not have any particles below 132 μm . A varied bond strength across the wheat kernel might result in a lower deviation from the lab milling results.

3.1.1. Sensitivity analysis of the sphere-shaped model

The sensitivity analysis was performed for simulations of 1st break milling at 16% moisture content. For shear modulus, it was found that the minimum value at which the model could simulate the milling process was 10 MPa. For simulations with a shear modulus value of 40 MPa and lower, it was found that the particle bonds break before the particle cluster came in contact with the break rolls (Fig. 6). In addition, the particle-bond system began to break when the clusters came in contact with other clusters and with the walls of the feeder. So, the simulation results below 50 MPa were not considered for comparison purposes and are not presented here. A shear modulus value of 50 MPa resulted in the least deviation in prediction of particle size from milling validation trials while also predicting the least mean geometric particle size for the same. With increasing shear modulus from 50 to 70 MPa, the mean geometric particle size increased as well (Table 5). However, this also resulted in increasing the mean relative deviation of the predictions. Since, the objective of sensitivity analysis was to decrease the percent deviation in prediction of particle size from lab scale validation results, a milling trial at 65 MPa was also simulated. Although results from the simulation at 65 MPa did not fall in the observed trend as seen from other trials (Table 5), it was observed that the deviation in prediction for this model decreased considerably. So, a shear modulus value of 65 MPa was selected for future simulations.

After calibrating the shear modulus to 65 MPa, the coefficient of restitution (COR) was decreased starting from 0.3 in decrements of 0.05. Similar to the observations made for model

simulations with shear modulus values of 40 MPa and lower, for COR values below 0.2 the particle bonds of the cluster started breaking before it came in contact with the break rolls. As the kernels were being fed into the break rolls from the hopper, due to the particle-particle contact and contacts with the hopper geometry, the bonds began to break. At a COR value of 0.25, there was an increase in the mean geometric particle size even though the mean relative deviation increased as well. At 0.3 COR, the particle size was similar to that of obtained at a COR value of 0.31. A study by Metzger and Glasser [18] investigating the effect of coefficient of restitution on breakage of agglomerates among other particle parameter, reported that at lower values of COR, the agglomerates tend to break up more easily since they tend to lose the majority of their energy and deform easily. This is possibly the reason why below certain values of COR and shear modulus the clusters tend to break with minimal contact.

3.2. Kernel-shaped approach

In this model, the exact shape of the wheat kernel was approximated using multi-layered spheres. In addition, bond strength varied across the kernel to depict the varying strength between the endosperm and bran layer. The bond strength ranged from 8.75×10^7 to 1.1275×10^8 N/m² for normal and shear stiffness with a critical normal and shear stress of 1.275×10^7 Pa. The model predicted a mean geometric particle size of 413 μ m for HRW wheat milled at 16% moisture content. Table 6 shows the cumulative distribution comparison of the results obtained from the model prediction and lab scale validation trials at 16% moisture content.

Similar to the sphere-shaped approach, the majority of the particles were within the range of 132 to 1041 μ m. The custom factory of 1st break fraction particles created the cluster comprised of particles with diameters ranging from 47 to 1387 μ m. However, as the clusters came in contact with the break rolls the cluster broke into the individual particles. The magnitude

of the forces from the roll exceeded the bond strength of the particle-bond system. The BPM characterized the bond created between particles in such a way that if the magnitude of the force acting on the particles was greater than any of the bond strength parameters given to the model, the particle-bond system broke, as was observed in this case. From Table 6, it was evident that the major difference was the fraction of material collected at 869 μm sieve opening. The DEM model, similar to the lab scale milling results, predicted minimal flour production during 1st break. However, the result from the model deviated by nearly 50% from the percent mass collected over the 869 μm sieve.

Though the predictions were better than with the sphere-shaped approach, the high percent deviation indicated that the bond variation assumed in this kernel-shaped approach did not exactly represent the kernel structural and strength characteristics. The problem with this approach was that the model randomly distributed the bond strength. But, in a wheat kernel, this strength follows a distinct pattern across the layers of bran and endosperm. So, the bonds are stronger in some sections of the cluster and a random distribution did not capture this pattern of variation in bond strength. The kernel-shaped DEM approach of predicting 1st break milling of HRW wheat was extended to simulate the milling process at 12 and 14% moisture content levels. The results for the model prediction at these moisture levels are summarized in Table 6. It was observed that with increasing moisture content, the mean particle size predicted by the model decreased, following a similar trend as displayed by the lab scale milling results (Table 6).

Even though the overall trend observed for model prediction and lab scale validation milling was similar, the mean relative deviation was very high. There was a high deviation in prediction, approximately 50%, for the percent mass of ground wheat collected over the 132 μm sieve opening, which was mainly due to the near complete breakage of the cluster only into small

fractions, individual particles, with few larger cluster fractions predicted. Studies that involved simulating fracture mechanism of agglomerates by making use of bonded/multi-layered particles [13, 33, 34] were able to predict the particle size of fractured particles in close agreement with experimental observations.

4. Conclusion

This study simulated the 1st break wheat milling process using the DEM modeling technique, which had not previously been used to simulate the size reduction of wheat kernels using a roller mill. Two different particle models were used, a sphere-shaped model with uniform bond strength and a kernel-shaped model with randomly distributed bond strength. Even though the sphere-shaped model had a large deviation from the experimental milling results, the model was able to correctly predict the trend observed for change in particle size of 1st break stream with moisture content. Using a sensitivity analysis, the optimum shear modulus and coefficient of restitution values were determined. The sphere-shaped model resulted in a better prediction at 65 MPa shear modulus value and at 0.31 COR. While both models successfully predicted the trends with moisture content, a relatively large deviation in prediction of particle size was observed compared to the experimental results. Future research could improve the model predictions by accounting for a distributed bond strength that better represents the wheat kernel in terms of its structural components; endosperm, bran layers, and germ; to enable breakage of the particles in a manner more similar to breakage of wheat kernels during the milling process.

Nomenclature

$\bar{F}^n$	Axial directed force
$\bar{F}^s$	Shear directed force
$\bar{M}^n$	Axial directed momentum
$\bar{M}^s$	Shear directed momentum
$\bar{\sigma}_c$	Critical tensile stress
$\bar{\sigma}_{max}$	Maximum tensile stress
$\bar{\tau}_c$	Critical shear stress
$\bar{\tau}_{max}$	Maximum shear stress
$\bar{R}$	Parallel bond radius
U^n	Relative displacement in the axial direction
U^s	Relative displacement in the shear direction
θ^n	Rotation component in the axial direction
θ^s	Rotation component in the shear direction
A	Area of the parallel bond
BPM	Bonded particle model
DEM	Discrete element method
HRW	Hard red winter
I	Moment of inertia of the parallel bond
J	Polar moment of inertia of the parallel bond
N	Number of observations
PSD	Particle size distribution
Y	Experimental value
Y_p	Predicted value

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Mention of trade names or commercial products in this article is solely for the purpose of providing specific information and does not imply recommendation or endorsement by the U.S. Department of Agriculture. USDA is an equal opportunity provider and employer.

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Figure Captions

Figure 1: 1st break roll geometry

Figure 2. Creating particles by spherical-shaped approach (A & B) and kernel-shaped approach (C & D)

Figure 3. Bonded particle cluster breakage at consecutive time steps during milling

Figure 4. Bonded particle cluster (A) before breakage (B) during and after breakage and (C) breakage of particle bonds during milling at consecutive time steps

Figure 5. Particle size distribution of simulation and validation samples

Figure 6. Breakage of bonding in particle cluster at a shear modulus of 40 MPa

Figure 1: 1st break roll geometry

Figure 2. Creating particles by spherical-shaped approach (A & B) and kernel-shaped approach (C & D)

Figure 3. Force-displacement behavior of particle bond system; B) parallel bond formation between two particle with resultant force s well and normal and shear torque (modified from [13])

Figure 4. Bonded particle cluster (A) before breakage (B) during and after breakage and (C) breakage of particle bonds during milling at consecutive time steps

Figure 5. Particle size distribution of simulation and validation samples

(Note: In the chart above, “\\” – Sphere-shaped approach; “=” – Kernel-shaped approach; “| |” – Lab scale validation. Blue – 16% mc; Orange – 14% mc; Green – 12% mc)

Figure 6. Breakage of bonding in particle cluster at a shear modulus of 40 MPa

Table 1. 1st break roller mill dimensions used in the simulation

Roll diameter, mm	250
Roll length, mm	800
Roll gap, mm	0.05
Roll speed, fast/slow, rpm	350/140
Speed differential, fast:slow roll	2.5:1
Grinding action	Dull-to-Dull
Flutes on circumference	350
Flutes per centimeter	4.5

Table 2: Physical and mechanical property values used as input parameters for particles and break rolls

Moisture content, % w.b.	Particle size, μm	Particle density, kg/m^3	Poisson's ratio	Shear modulus, MPa	Coefficient of restitution	Coefficient of static friction	Coefficient of rolling friction
<i>Wheat kernel</i>							
12	1275 (± 200)	1423	0.20	76.5	0.33	0.38	0.19
14	1295 (± 200)	1420	0.20	76.5	0.32	0.39	0.19
16	1305 (± 205)	1416	0.20	76.5	0.32	0.40	0.20
<i>1st break stream</i>							
12	283	1453	0.20	76.50	0.27	0.33	0.17
14	296	1450	0.20	76.50	0.30	0.36	0.18
16	400	1431	0.20	76.50	0.31	0.37	0.23
<i>Roll stand, steel</i>							
	-	7800	0.30	77000	-	-	-

Table 3. Particle bonding parameters

Bond parameters	Critical value
<i>Single Sphere Approach</i>	
Normal stiffness*, N/m ³	1 x 10 ⁸
Shear stiffness*, N/m ³	1 x 10 ⁸
Normal stress*, Pa	1.275 x 10 ⁷
Shear stress*, Pa	1.275 x 10 ⁷
Bond radius, mm	1
Bond start time, s	0.29
<i>Multi Sphere Approach</i>	
Bond formation time, s	0.29
Single sphere contact radius, %	75
Particle	Fraction
Normal stiffness*, N/m ²	1 x 10 ⁸ +/- 1.275 x 10 ⁷
Shear stiffness*, N/m ²	1 x 10 ⁸ +/- 1.275 x 10 ⁷
Critical normal stress*, Pa	1.275 x 10 ⁷
Critical shear stress*, Pa	1.275 x 10 ⁷
Bond disk scale	1

Table 4. Average particle size of milled and simulated particles

Moisture content, % wet basis	Mean geometric particle size (μm)		Mean relative deviation
	DEM model prediction	Lab-scale results	
12	413 (± 172)	808 (± 488)	185%
14	410 (± 169)	787. (± 500)	175%
16	438 (± 202)	751. (± 511)	177%

* Values in parenthesis are standard deviation

Table 5. Sensitivity analysis for sphere-shaped model

Shear modulus (MPa)	Mean geometric particle size (μm)	Mean relative deviation*
	DEM model	
50	368 (± 105)	142%
60	423 (± 184)	170%
65	372 (± 111)	144%
70	435 (± 199)	175%
76	438 (± 202)	177%
Coefficient of restitution with a shear modulus of 65MPa		
0.25	382 (± 128)	149%
0.30	375 (± 132)	146%
0.31	372 (± 111)	144%

* Deviation from the particle size of 751 (± 511) μm obtained through lab scale milling trials at 16% moisture content.

** Values in parenthesis are standard deviation.

Table 6: Particle size comparison at different moisture content

Moisture content, % wet basis	Particle size (μm)		Mean relative deviation
	DEM model prediction	Lab scale milling results	
12	466 (± 241)	808 (488)	138
14	456 (± 228)	787 (500)	158
16	413 (± 178)	751 (511)	139

* Values in parenthesis are standard deviation