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DEM Model of Wheat Grains in Storage Considering the Effect of Moisture Content in Direct Shear Test

[1]Hamed Johnny Sarnavi, [2]A. Noor Mohammadi, [2]A. Modares Motlagh and [2]A. Rahmani Didar
[1]Member of Young Researchers Club, Khorramabad Branch, Islamic Azad University, Khorramabad, Iran
[2]Department of Mechanic of Agricultural Machinery Engineering, Urmia University, Urmia, Iran

Abstract: Discrete Element Method (DEM) modeling was conducted for predicting strength properties of stored wheat grains in different levels of moisture contents, to extend the knowledge of grain storage beyond current experimental studies in the future. The main features of agricultural and food materials that make them different from mineral materials are strong influence of Moisture Content (MC) on mechanical behavior. Published data on grain and bulk properties of wheat relevant to DEM modeling were reviewed by considering the effect of MC. The shape of grains was modeled by Multi Sphere Method (MSM) and the interaction between grains was represented by linear and nonlinear frictional elastic contact models. The effect of MC was considered in simulation through an innovative procedure. The initial test was performed to choose the best models to perform the simulation. Statistical comparisons with relevant experimental result were conducted on simulation data. It has been proved that the DEM is able to capture the variation of strength properties of wheat with MC of grains. It is observed the simplest shape of grain models would allow us to obtain quite closely prediction of wheat strength parameters. Also the linear elastic contact model has more capability in representing the form of strength properties variation with MC. This suggests that the modeling is a useful tool in the study of mechanical behavior of wheat and other cereal grains during storage processes as well as provision of data necessary in the future design of appropriate machinery and structure.

Keywords: Cohesion, discrete element method, friction coefficient, internal friction angle, moisture content, simulation, wheat

INTRODUCTION

For many years vast quantities of cereal grains and other agricultural products have been stored in silos like other mineral and engineering materials. The storage of granular solids in silos provides many interesting problems concerning pressures and flow (Rotter *et al*., 1998). Mechanical properties of agricultural seeds are needed for appropriate design of processing machines but its specific application should be understood before determining them experimentally (Mohsenin, 1986). Thus, an appropriate model for predicting storage of grains will be valuable. Important flow properties of bulk grains are modulus of elasticity, Poisson ratio, internal friction angle, apparent cohesion. The measurement of these properties lets the engineer design and optimize storage systems and processing plants of grains (Molenda and Stasiak, 2002; Stasiak *et al*., 2007). There are different codes to study the bulk properties of particulate material, like ASTM and Eurocodes (ASTM-D6128, 2000 and Eurocode 1, 2003). Code of practice usually contains standard procedures for determination of bulk properties of stored grains. A comprehensive understanding of the bulk behavior for biomass can be attained if a modeling study is conducted. Thus, a valid comprehensive model for predicting bulk behavior of grains will be valuable for extending the knowledge of grain storage beyond current experimental studies. Bulk handling behavior of the grains can be studied experimentally, but large-scale investigations of grain flow can be expensive and time consuming (Boac *et al*., 2010). With increasing speed of computers, the DEM is becoming gradually a more effective technique for the simulation of particulate material in the area of biomaterials as well as engineering materials (Abbaspour-Fard, 2004). Actually computer simulations provide a cost-effective alternative to physical experimentation. The main features of agro and food materials that make them different from mineral materials are strong influences of MC on mechanical behavior and high deformability of grains. These differences bring about certain peculiar behaviors and necessity of adjustments of models of material, experimental techniques and technological solutions (Molenda *et al*., 2004). It can be seen that increasing the MC causes notable increases of pressure on silo walls. Because the increase of pressure requires an increase in the thickness of silo construction

Corresponding Author: Hamed Johnny Sarnavi, Member of Young Researchers Club, Khorramabad Branch, Islamic Azad University, Khorramabad, Iran

materials, costs of construction increase. Also, flow problems in silos such as arching, ratholing, irregular flow and segregation occur with increased MC (Kibar *et al*., 2010). Molenda and Horabik (2005) mentioned that according to Canadian Farm Building Code, increase in MC of stored grain may result in a six fold increase in pressure acting on silo wall. DEM could be very potential to recognize and embed the effects of MC in simulation, because of its intrinsic character which simulate bulk solids properties through material and interaction properties of grains. Mani *et al*. (2003a, b) model the compaction behavior of corn stover grinds in the densification process, they used the damping models to take the effect of MC into account. Stasiak and Molenda (2004) examine the influence of MC of two groups of food powders on their angles of internal friction and strength characteristics.

In this study, first, published physical and mechanical properties of wheat grains needed to model grain flow in DEM were reviewed and then interaction properties between grains that will represent in form of contact models were pursued. Therefore an appropriate model for Wheat, based on appropriate relevant properties, would be developed and valid. Wheat was chosen as the test grain due to its superabundance in agriculture all over the world. Validation was accomplished through comparison of acquired test simulation data with respective experimental result.

Properties of grains: An important issue in the DEM modeling is the characterization of the grains which, in general, have different shapes and sizes and rheological properties. Moreover, each of these rheological properties depends on the amount of MC of grain (Zhu *et al*., 2007). The applied parameter in DEM can be divided into two categories: material and interaction properties (Raji and Favier, 2004a, b). Kibar *et al*. (2010) investigate some physical and mechanical properties of a variety of rice regarding the effect of MC. All of these properties will be affected by amount of MC. Al-Mahasneh and Rababah (2007) measured physical properties of green wheat over MC range from 9.3 to 41.5% which covers the moisture range from harvesting to storage.

In the DEM modeling, shape is one of the most important physical and geometrical properties of grains. To demonstrate the shape of wheat grains, some dimensions of grain have been measured and published in many studies (Nelson, 2002; Molenda and Horabik, 2005; Al-Mahasneh and Rababah, 2007).

Molenda *et al*. (2004) reported mean grain size of many selected ground feedstuffs in five levels of MC. Also, the authors measured mean values of grain dimensions of wheat. The measured dimensions for wheat are cited in Table 1. Nelson (2002) determined seed mass, volume, density and dimensions for five varieties of wheat in different levels of MC (8.6-16.9%). Molenda and Horabik (2005) determined the mass of 1000 seeds for wheat. Al-Mahasneh and Rababah (2007) presented two regression equations for relationship between mass of 1000 seeds and value of MC and also between volume of seed and value of MC, which the first was shown in Table 2. Arnold and Roberts (1969) examined seven varieties of wheat, having MC in the range of 11.5-13%, to determination modulus of Elasticity (E). Elastic Module of wheat falls within the range of 1.46-2.83 GPa depend on MC and verity. Glenn *et al*. (1991) reported Elastic modulus of wheat, determined for cylindrical samples cored from the grain endosperm, in the range of 0.2-3 GPa depending on the variety. Also Delwiche (2000) stated that with increasing Mc value of grains, its Elastic modulus decrease to stabilize at MC levels above 22%. Khodabakhshian and Emadi (2011) reported some published value of elastic modules for some verities of wheat in different levels of Mc by Shpolyanskaya (1952), Zoreb and Hall (1960) and Shelef and Mohsenin (1969) (Table 1). According to ASABE Standards (2006) Poisson's ratio (ν) falls within 0.16-0.42. In a study on wheat that was done by Shelef and Mohsenin (1969), Poisson's ratio was assumed 0.4. Arnold and Roberts (1969) have investigated the effect of deformation and elastic modulus on Poisson's ratio of wheat. They revealed that variation of Poisson's ratio of wheat was 0.3 to 0.5. Many researchers have also assumed a value of 0.4 for Poisson's ratio of agricultural products (Fridley *et al*., 1968; Arnold and Roberts, 1969; Shelef and Mohsenin, 1969). Kibar *et al*. (2010) revealed that the poisons ratio of the rice grain decreased linearly with the increase of MC. The highest value (0.34) for poisons ratio at 10% MC, the lowest value (0.32) was recorded at 14% MC. Shear modulus (G) defined in term of poison's ratio (ν) and modulus of Elasticity (E) is given as follows (Mohsenin, 1986):

$$G = \frac{E}{2\,(1+\nu)} \tag{1}$$

Molenda and Horabik (2004) determined the coefficient of friction between a wheat grains and a sliding surface with DST, they obtained mean values of the friction coefficient of wheat grain in the MC of 10-20% against stainless steel in different normal forces and the values corresponding to normal stress of 60 kPa are listed in Table 3, the authors also reported mean internal coefficient of friction for wheat at MC percentage of 10, 12, 14, 16 and 18. Benedetti and Jorge (1979) determined coefficients of friction for grain-grain and grains-steel in four levels of MC (Table 1). Brubaker and Pos (1965) reported that the static coefficient of

Table 1: Published material and interaction properties of wheat grains

Wheat grain property	Reference	Moisture contents (%)	Values
Material properties			
Dimension:			
Length (mm)	Nelson (2002)	8.6-16.9	L: 5.6~6.9 W: 2.6~3.4 Th: 2.4~2.9
Width (mm)	Al-Mahasneh and Rababah (2007)	9.3~41.5	L: 6.24~6.66 W: 3.65~4.22 Th: 3.43~3.85
Thickness (mm)	Molenda and Horabik (2005)	10	L: 6.7 W: 3.2 Th: 2.9
Density (kg/m^3)	Nelson (2002)	8.6-16.9	1345~1411 (1369)[2]
	Molenda and Horabik (2005)	10	1407
Volume (mm^3)	Al-Mahasneh and Rababah (2007)	9.3~41.5	28.84~41.95
	Nelson (2002)	8.6-16.9	18.5~28.6 (24.4)[2]
Mass (gr) (1000 seeds)	Al-Mahasneh and Rababah (2007)	9.3~41.5	32.57~51.95
	Molenda and Horabik (2005)	10	40.50
	Nelson (2002)	8.6-16.9	26.00~39.70 (33.4)[2]
Interaction properties			
Modulus of elasticity (GPa)	Arnold and Roberts (1969)	11.5~13	1.46~2.83
	Glenn *et al*. (1991)	0~30	0.2~2.8
	Shelef and Mohsenin (1969)	10	1.08~2.86[3]
	Zoreb and Hall (1960)	11~15.7	0.08~6.52[3]
	Shpolyanskaya (1952)	11~12	2.94
Poisson's ratio	Arnold and Roberts (1969)	-----	0.3~0.5
	Fridley *et al*. (1968)	-----	0.4
	Shelef and Mohsenin (1969)	-----	0.4
	Kibar *et al*. (2010)	10~14%	0.34~0.32[4]
Coefficient of friction*	Molenda and Horabik (2005)	10~20	grain-steel: 0.16~0.287 (normal stress = 60 kPa)
	Benedetti and Jorge (1979)	10~25	grain-grain: 0.16~0.287 grain-steel: 0.595~0.833
	Brubaker and pos (1965)	11.2~15.7	grain-steel: 0.10~0.33

1: Static coefficient; 2: Reported mean value; 3: By different method; 4: For rice grains

Table 2: Regression equations to initialze input parameters of DEM model, in terms of moisture content

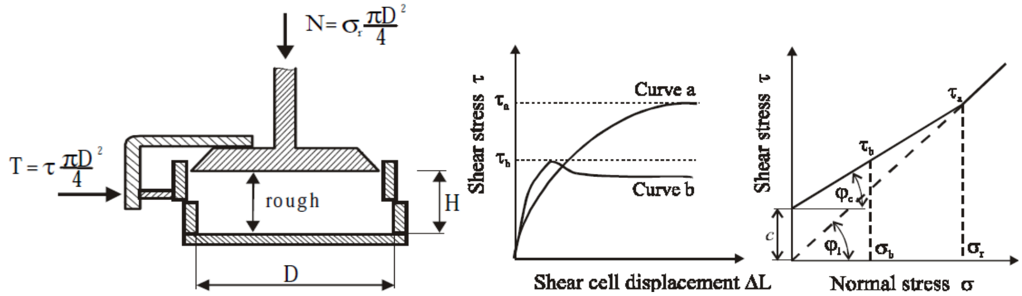
Input parameter	Equation of trend line (regression coefficient)	References
Mass (gr) (1000 seeds)	$M_{1000}(gr) = 0.592\ \mathrm{MC} + 26.684\ \ (\mathrm{R}^2 = 0.98)$	Al-Mahasneh and Rababah (2007)
Friction coefficient (grain-grain)	$\mu_{g-g} = 0.001\mathrm{MC}^3 - 0.054\mathrm{MC}^5 + 0.899\mathrm{MC}\ 4.017\ (\mathrm{R}^2 = 1)$	Benedetti and Jorge (1979)
Poisson ratio	$\nu = -0.005\mathrm{MC} + 0.385\ (\mathrm{R}^2 = 0.98)$	Kibar *et al*. (2010)
Elastic module (GPa)	$\mathrm{E} - 0.178\ \mathrm{MC} + 4.405\ (\mathrm{R}^2 = 0.97)$	Glenn *et al*. (1991)

Table 3: Input parameters of DEM model in five levels of moisture contents

							Shear stiffness (kN/mm)		Normal stiffness (kN/mm)	
MC (%)	Bulk porosity (%)	Mass 1000 seeds) g	Elastic module (grain kernel) GPa	Poisson ratio (grain kernel)	Friction coefficient (grain-grain)	Friction coefficient (grain-steel)	Spherical	Multi sphere	Spherical	Multi sphere
10.0	49.8	32.568	2.625	0.335	0.573	0.160	16.607	12.791	20.790	16.013
12.5	48.8	34.048	2.180	0.323	0.736	0.163	13.946	10.741	17.266	13.298
15.0	50.9	35.528	1.735	0.310	0.693	0.182	11.221	8.642	13.741	10.584
17.5	52.8	37.008	1.290	0.298	0.537	0.287	8.431	6.494	10.217	7.8690
20.0	54.3	38.488	0.845	0.285	0.363	0.279	5.580	4.298	6.6920	5.1550

friction was significantly influenced by the MC of the grains and test surface. These authors suggested that after exceeding 13% of MC of grain a particularly fast increase in friction took place. The static coefficient of friction, in general, increased with the MC of the grain (Benedetti and Jorge, 1979; Lawton, 1980; Horabik *et al.*, 1991). Benedetti and Jorge (1979) determined internal coefficients of friction for wheat grains at various MCs, which were between 0.590 and 0.833.

Bulk properties of grains: Strength parameters of internal angle friction (φ) and apparent Cohesion (C) of particulate material influence handling and processing operations such as flow from silos and hoppers, transportation, mixing, compaction or packaging (Knowlton *et al.*, 1994). To obtain a quantitative statement regarding the flow behavior of a bulk solid, a defined measurement of strength properties is required following the standard tests Kibar *et al*. (2010)



(a) (b)

Fig. 1: Jenike shear tester and its relevant diagram: (a) Jenike shear tester, (b) relevent diagram of shear test

Table 4: Published bulk properties of wheat grains measured by Molenda and Horabik (2005)

	Internal angle of friction (degree)		Cohesion (kPa)		
Moisture content (%)	Mean	S.D.[1]	Mean	S.D.	Porosity (%)
10.0	25.7	0.3	0.9	0.5	49.8
12.5	26.2	0.4	2.8	0.5	48.8
15.0	27.0	0.5	2.1	0.7	50.9
17.5	33.0	1.0	5.1	0.5	52.8
20.0	35.5	0.5	2.3	0.9	54.3

[1]: Standard Deviation

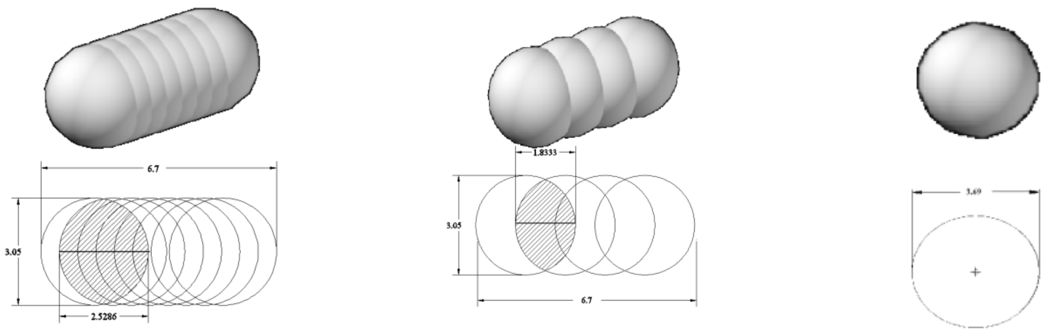
reported a positive linear relationship between the MC and internal angle of friction for rice grains. Molenda *et al*. (1998) also found in their study that the angle of internal friction increased linearly with increase of MC for wheat grains. Numerous granular materials when consolidated reveal cohesion that allows maintaining shape enforced under load (Molenda and Horabik, 2005).

The DST has been frequently used to measure frictional properties of granular materials because of its simplicity and versatility. This test is usually performed by a pair of circular or square cells in which a particulate test sample is sheared to failure by the application of a lateral shear force (Fig. 1). Molenda and Horabik (2005) used DST recommended by standard of the (ASTM-D6128, 2000; Eurocode 1, 2003). The apparatus consists of the lower ring, the upper ring and the base. The lid of the shear cell is loaded with vertical force N and then lateral displacement is applied on a bracket attached to the lid. This test creates a shear zone within the assembly of grains by the relative movement of one cell with respect to the other. Shear tests performed again with identically consolidated samples under defined normal loads give respective shear forces (For more details refer to Molenda and Horabik (2005). Molenda and Horabik (2005) measured the bulk and strength properties of wheat in five levels of MC (Table 4).

MATERIALS AND METHODS

DEM modeling: The three dimensional Discrete Element Method (DEM) model was applied for simulation of the wheat grains in DST by Particle Flow Code (PFC) from Itasca software version 3.1. DEM is a numerical modeling method that makes use of contact mechanics between the particles to model the mechanical behavior of assemblies of particles (Kremmer and Favier, 2001a, b). The DEM is based on the Lagrangian approach, used to track the position, velocity, orientation and other parameters of particles during simulation (Dziugys *et al*., 2005). Newton's law of motion gives the relationship between particle motion and the forces acting on each particle. PFC^{3D} models the behavior of particles, which may be enclosed within a finite volume by non-deformable walls. Two basic structural elements exist in this code, ball and wall. The Newton's law of motion is applied for balls in each time step, during simulation, neither for walls. Walls allow one to apply velocity boundary conditions to assemblies of balls for purposes of compaction and confinement (Itasca, 2006). The balls and walls interact with one another via the forces that arise at contacts. So the walls would have an independent motion during simulation and therefore would be very suitable to simulate the strain controlled test.

Grains used in various engineering fields often have very irregular shapes and this grain shape greatly affects the mechanical behavior of their assembly. Therefore adequate grain shape modeling is quite important in DEM simulation for quantitative discussion (Matsushima *et al*., 2003) By MSM, a number of spheres can be joined together to create a model of grains shape in DEM modeling (Abbaspour Fard, 2004). It is also possible in the PFC^{3D}, to create



$l = 6.7\ mm, d = 3.05\ mm, x = 2.5286\ mm$

(a)

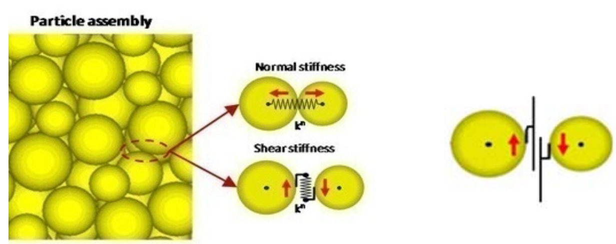
$l = 6.7\ mm, d = 3.05\ mm, x = 1.8333\ mm$

(b)

$d = \text{Mean Diamete} = \sqrt[3]{6.7 \times 3.2 \times 2.9} = 3.96\ mm$

(c)

Fig. 2: MSM models of wheat grains a) 8 spheres grain, b) 4 spheres grain, c) Spherical grain Dimensions based on published data by Molenda and Horabik (2005)



$F^n = k^n U^n$
$\Delta F^s = -k^s \Delta U^s$

(a)

$F^{Slip} = \mu |F^n|$

(b)

Fig. 3: Frictional elastic contact models: (a) Elastic model (normal and tangential), (b) Frictional model (slip)

grains of arbitrary shape by attaching two or more balls together and each group of particles acts as an autonomous object (Itasca, 2006).

The shape of wheat grains has been modeled by spherical surfaces of balls. Three types of grain created in modeling: Spherical, 4-Spheres and 8-Spheres by MSM. The dimensions of each type were given on the basis of wheat grain size that published in the literature (Molenda and Horabik, 2005). The geometrical properties of them were demonstrated in Fig. 2. The three dimensions of wheat grains (length, width and thickness) were derived from Table 1 and their variation with MC was considered negligible.

Contact force models hold the key to accurate DEM simulations. They are required to be as simple as possible to limit computational complexity while providing an accurate estimation of the force-deformation Relationship. For a majority of DEM applications and for agricultural products in particular, simple but accurate contact force models are a challenge that needs urgent attention to allow achievement of the desired accuracy of the DEM models (Dintwa *et al*., 2003). Regarding contact models, there is an extensive literature for elastic spheres (Mindlin, 1949; Mindlin and Deresiewicz, 1953; Walton, 1987; Walton and Braun, 1986; Brilliantov *et al*., 1996). Almost all of these works used the theory of Mindlin (1949) which gives the tangential force-deformation relationship of contacting spheres as dependent on the normal force F_n; the material surface properties (friction coefficient) as well as the material elastic properties (shear modulus G and Poisson's ratio v). The normal contact force is deriving from Hertz's theory (Johnson, 1985) too.

The overall force in each contact between particles, called unbalanced force, is composed of two perpendicular force components; the normal and the tangential as well as other body force like gravity weight. Also there is an unbalanced moment at each ball. These unbalanced force and moment could be used as a criterion to reach a stable state, in the assembly of balls. As in this study in preparing the sample, stable state is achieved when the ratio of unbalanced force to contact force for all balls reaches the value of 0.01.

In DEM research a distinction has to be made between soft and firm biological materials. The contact between wheat grains classified as firm one and in silo condition or during handling, the firm material usually deformed as dense granular material. In firm models, it is assumed that the interaction forces between grains are impulsive. Moreover the dominant force in dense granular flow is friction, so the frictional contact model could be adequate. Most research has been done on firm biological materials. Van Zeebroeck (2005) study the apple bruises as a soft material contact, he also recount some of the work on firm biological material: Rong *et al*. (1995), Jofriet *et al*. (1997), Lu *et al*. (1997), Negi *et al*. (1997), Raji and Favier (1998), Rotter *et al*. (1998), Holst *et al*. (1999), Kremmer and Favier (1999) and Raji and Favier (1999, 2004). In this study the contact model acting at each contact consists of two parts: stiffness model and frictional model, which were shown in Fig. 3. The stiffness model provides an elastic relation between the contact force and its corresponding deformation. The frictional model enforces a relation between shear and normal contact forces such that the two contacting balls may slip relative to one another. This Frictional Elastic model is defined by the normal stiffness (k_n) and shear stiffness (k_s) as well as friction coefficient (μ) (Fig. 3). When the value of stiffness is independent of force and deformation and has constant value during contacts, it means linear elastic model. But when values of stiffness have changed by amount of deformation during contacts, it would be a nonlinear elastic property Eq. (4) and (5). The input parameters of the contact models were derived from wheat kernels properties in different levels of MC. The determination of the stiffness values is somewhat critical and complex. Landry (2005), mentioned the fact that the method for the evaluation of the parameters in the linear model has received very little attention in the literature. Di Renzo and Di Maio (2004) proposed a method to calculate the ratio (K) of tangential stiffness (k_s) to normal stiffness (k_n) for two same particle:

$$\frac{k_s}{k_n} = \frac{1-\nu}{1-0.5\nu} \tag{2}$$

where, ν is the Poisson ratio of the particle.

It has also been suggested (Itasca, 2006) that the stiffness (kN/mm) could be determined using the following equation:

$$k_n = 4ER_{ball} \tag{3}$$

where,

R_{ball} : The radius of the particle (mm)
E : The elastic module (GPa)

So the radius of composing ball (Fig. 1) was applied to obtain the stiffness properties of wheat grain kernels ($R_{ball} = 3.05$ mm for multi sphere grains and $R_{ball} = 3.96$ mm for spherical grains).

The simplified Hertz-Mindlin model was applied to simulate wheat grains contact. This non-linear contact model defined by the shear modulus (G) and the Poisson's ratio (ν) of wheat grain kernels, which reviewed in literature for different MCs (Table 1):

$$k^n = \frac{2G\sqrt{2R}}{3(1-\nu)}\sqrt{U^n} \tag{4}$$

$$k^s = \frac{2\sqrt[3]{3(1-\nu R)G^2}}{2-\nu}\sqrt[3]{|F^n|} \tag{5}$$

Considering the effect of moisture content: DEM bridges the gap between macroscopic and microscopic models (Markauskas and Kačianauskas, 2006). As a matter of fact, DEM results macro properties through micro properties by numerical calculation techniques. So when an issue like MC of wheat grains affects its bulk behavior, we can expect changing the micro properties based on the amount of MC, would result macro properties at respective MC level.

The micro properties of wheat grains that were used in this modeling, include grain dimensions, density, mass, volume, Poisson ratio, Elastic modules, Coefficient of friction (grain-grain and grain-steel) and the macro properties were the strength parameters of wheat grains mass, which would be derived in DST. This kind of MC simulation would allow us to assess the direct effect of grain MC on its mass properties, but it needs to have the measured values of input parameters at the specific range of MC. So it remains a challenge of lacking fit published data. To surmount this challenge, the equation of best polynomials trend line which could estimate the change of process with the MC, was applied for each input parameter of DEM model that we have not their values at specified levels of MC. The change of wheat grains dimensions with MC is not significant, so the wheat grain shape were the same at different levels of MC and the measured values for Begra variety of wheat by Molenda and Horabik (2005) were used here. The values of mass, friction coefficient (grain-grain), poisons ratio and elastic module of wheat grains, were calculated for five levels of MC by regression equations, which respectively obtained from results of Al-Mahasneh and Rababah (2007), Benedetti and Jorge (1979), Kibar *et al.* (2010) and Glenn *et al*. (1991) (Table 2). The measured values of friction coefficient between grains and steel by Molenda and Horabik (2005), in the normal stress of 60 kPa, were used to grain models (these values were shown in Table 3). The regression equation of rice kernel poison ratio was applied, whereas there was no data in reviewed published studies for wheat grains (Table 2). The density of each type of grain model calculated through dividing mass of a grain by its volume. The volume of each grain is equal to occupied space of shear cell by that grain model.

Direct shear test simulation: The Jenike method of DST allows the determination of internal angle of friction and cohesion. Euro code 1 recommends using a simplified Jenike method (including consolidation and shearing of the sample) for the determination of strength parameters. The shear cell Diameter (D) should be at last 20 times the maximum particle size and not less than 40 times the mean particle size. The height H should be between 0.3 and 0.4 D. The sample should be poured into the test cell, without vibration or other compacting forces and then the consolidation stress σ_r should applied (Molenda and Horabik, 2005). Numerical simulations were carried out under the same conditions as the experimental tests. In this study, DST simulation is based on the test performed by Molenda and Horabik (2005) to determine flow properties of wheat grains mass in five levels of MCs. Comprehensive Procedure of this test has been published in ref (Molenda and Horabik, 2005) in details. Dimensions of the shear cell and other specifications of this test were shown in Table 5.

At first the rigid cylindrical walls (upper and lower ring of shear) as well as a flat wall (bottom of cell) were introduced in simulation software with their real dimensions to establish model. The grain creation algorithm was written using the FISH programming language, which embedded in the PFC^{3D} software package (Itasca, 2006). To have a similar specimen as same as the real one, the porosity values of wheat Assembly (Table 2) has used to calculate the approximate required number of wheat grains. Then after producing a specified number of shrieked balls in the shear cell space, the balls have been launched to enlarge pending to reach their final size and the required porosity was achieved. In the meantime the gravity acceleration was applied to the balls gradually to sediment the assembly. The contact model defines in this stage with unreal input values, to the assembly reach stability sooner. As mentioned in the past, when the ratio of average unbalanced force to average contact force reach 0.01, it considered as stable state of the assembly. Therefore the lid of shear cell composed of chained balls (Itasca, 2006), would exerted an extensive force on the assembly lead to reference stress. This extensive force was gradually increased from zero to the required value. This chained balls is similar to the membrane used by Iwashita and Oda (2000) and Belheine *et al*. (2008), respectively in DEM simulation of drained Triaxial test and shear test (Belheine *et al*., 2008). By applying the lateral motion of top ring, the perfect strain control test could be commenced. In every test, at first the saved created specimen was called in software, then the reference stress was exerted and the shearing process had begun. The shearing process was continued by lateral motion of upper ring while the ratio of lateral displacement to diameter of shear cell ($\frac{\Delta l}{D}$) was approaching to a specified value.

When $\frac{\Delta l}{D}$ exceeds 0.05 (Molenda and Horabik, 2005), the existing lateral force exerted by grains on top ring was recorded. In this way, each test results two value of shearing force. By dividing these two values by shear cell section area ($\pi D^2/4$), the two shearing stresses were obtained (τ_a and τ_b):

$$\tau = \frac{F_{lateral}^{top\ ring}}{\frac{\pi D^2}{4}} \quad \left(\frac{\Delta l}{D}=0.05\right) \tag{6}$$

then According to these equations, the value of Internal Angle of Friction (φ) and Apparent Cohesion (C) would be calculated:

$$\varphi = \arctan\left(\frac{\tau_a - \tau_b}{\sigma_r - \sigma_b}\right) \tag{7}$$

$$C = \tau_a - \sigma_r \tan\varphi m \tag{8}$$

to have the best DEM model for grains it is necessary to choose an appropriate model which not certainly was modified at the input parameter to achieve more real results, because the farther the value of input

Table 5: The specification of direct shear test in simulation

Cell specification				Loading specification			
Height (H)	Diameter (D)	Elastic module	Poisson ratio	Strain rate (loading)	Principal reference stress (σ_r)	Consolidation reference stress (σ_b)	$\Delta l/D$[1]
80 mm	210 mm	200 GPa	0.25	10.8 mm/min	100 kPa	50 kPa	0.05

[1]: The ratio of lateral displacement to diameter of upper ring (defined by standards and codes)

Table 6: Simulation results of shearing forces in three repetition at the initial test

		Horizontal force acting on upper ring (N) Reference normal stress = 50 kPa			Reference normal stress = 100 kPa		
Frictional-elastic contact model	Shape	First	Second	Third	First	Second	Third
Linear	Spherical	1057.32	1048.25	1055.56	2014.72	1999.73	2008.38
	4-Spheres	1008.41	989.070	1006.64	1937.51	1899.54	1932.59
	8-Spheres	1006.60	998.380	1006.84	1929.67	1918.95	1934.53
Nonlinear	Spherical	1097.59	1043.45	1111.84	2063.93	1972.10	2080.20
	4-Spheres	1037.31	1012.85	1037.45	1981.16	1934.15	1966.81
	8-Spheres	1087.92	1025.63	1095.51	2080.64	1978.70	2098.04

Table 7: Simulation results of shearing stress at the initial test, comparison with respective experimental values

		Internal angle of friction (respective measured value = 27ºC)		Cohesion (respective measured value = 3.25 kPa)	
Frictional elastic contact model	Shape	Simulation result (S.D.)[1]	Probability level (%)[2]	Simulation result (S.D.)	Probability level (%)
Linear	Spherical	28.788 (0.328)	95.79	2.809 (0.327)	79.88
	4-Spheres	28.073 (0.874)	60.09	2.281 (0.208)	47.03
	8-Spheres	27.999 (0.649)	68.59	2.250 (0.263)	32.97
Nonlinear	Spherical	28.901 (1.875)	52.75	3.725 (0.683)	82.45
	4-Spheres	28.051 (1.368)	42.57	2.693 (0.705)	45.79
	8-Spheres	29.794 (1.967)	65.63	2.497 (0.661)	34.52

[1]: Standard Deviation; [2]: Corresponding t values were computed by $t = \frac{Population\ Mean - Sample\ Mean}{Standard\ Deviation\ of\ Sample \times \sqrt{\frac{n+1}{n}}}$, which proposed by Sokal and Rohlf (1995)

parameter from origin, leads to the less inherent modeling, however it would give good results at a specific condition. In summary, this work, which is restricted to wheat grains, must be viewed as the first step towards the building of a comprehensive and universal DEM based model considering intrinsic nature of grains. This study has been performed by comparison acquired simulation data with its relevant published result in the literature by Molenda and Horabik (2005), which were shown in Table 4.

RESULTS AND DISCUSSION

At first, six combination of contact model-shape (two types of contact models with three types of shapes) were surveyed to choose the most adequate combination model. Then the selected combination models have been used to study the ability of DEM model in predicting strength properties of wheat mass in different MC levels. Also DEM modeling was conducted to determine the linearity or nonlinearity of the elastic nature of wheat grains at contacts in mass, by using the material and interaction properties of wheat grains, based on values in the literature. The following discussion was drawn on the basis of statistical comparisons. Each simulated test would give two strength parameters of wheat grains: φ and C.

In each test the mean with standard deviation from expected values were determined from the values of φ and C, for three replications. Therefore to survey the validation of modeling, the obtained data compared with their corresponding experimental published values. Furthermore to compare two mean values, published and simulation values, probability levels under the t-test distribution curve for each simulated test results were determined. So the corresponding probability of the t would be the chances of model to predict the correct φ or C values, which the t was calculated for. Also to study the process of the change of φ or C with increasing wheat grains MCs and to show the goodness of the fit between two set of experimental and simulation values, the correlation coefficient of two set of numbers has been used.

Initial test: In the initial simulations, the input parameters corresponding to 15% MC were applied to modeling. In this test, it is observed that the simplest shape of model would allow us to obtain better results, but the type of contact model exerted a significant effect on the values. Boac *et al.* (2010) also stated that a single sphere particle model best simulated soybean kernels in the bulk properties test. As when spherical grains were applied with linear elastic model, φ would be predicted best, but for C it was not very notable and even nonlinear contact model gave better result. The multi sphere shape of grain would not rather than spherical grain, but the number of spheres affect the result as were shown in Table 6 and 7. These differences could be explained by pseudo friction effect that was mentioned by Markauskas and Kačianauskas (2006). They believed that it could be explained by additional friction between multi spheres grains. As the outer boundary of a multi-sphere model grain consists of spherical segments, during contact between two neighboring model grains, these segments can cause interlocking between the particles. Also it is worth noting that, neglecting linearity of models, by increasing the number of spheres the ability of predicting C decreased. It was confirmed that the linear models have an absolute excellence in comparison with nonlinear ones, in predicting φ values, while there is no considerable difference between linear and nonlinear models about C. Nonlinear models just when combine with spherical grains could reach acceptable probability level for representing experimental C values. In summary, by means of unmodified DEM simulations, predicting the φ values were conducted better than C values. The best estimate for both strength properties (φ and C) is obtained by the set of linear elastic contact model with spherical grain. Nevertheless the two spherical grain models were selected to assay simulation of the MC of wheat grains.

Moisture content simulation: The specific properties of wheat grains in different levels of MC were incorporated into the selected models, to represent realistic strength properties of assembly. The input parameters of both linear and nonlinear models were used as shown in Table 3. To discuss about simulation of DST for wheat grains, considering its MC, it was necessary to study obtained strength properties of wheat mass (φ and C) separately, because each of them has its variation form with MC. The linearity of contact model were also revised by comparison its results with each other.

Internal angle of friction: It was observed that, the φ values increase by MC increasing, like experimental result as was shown in Fig. 4. But there are some differences between the two ones, in simulation data we have a steady increasing of φ, while in experimental results, there is a sudden increase of φ that occurs between 15 and 17.5% of MC. Moreover the probability of correct prediction of Experimental φ values had been presented for five revised MC levels in Table 8. Altogether there is a high chance to prediction of φ values by linear contact model in five revised MC; this probability was 68.51% on average. The best chance refers to 15 and 10% of MC that are respectively equal to 94.51 and 90.77% and the worst ones refers to 17.5 and 20% of MC which respectively are 41.26 and 42.33%. The correlation coefficient for the simulation values against published experimentally values was equal to 0.98, in representing variation of φ by increasing MC for linear elastic contact model. This correlation coefficient was very satisfactory and the best among all in this study. It has been found that the prediction of φ by linear contact model was carried out better at lower MC in simulations.

With assuming nonlinear nature of contact in wheat grains assembly, just two acceptable predictions of apparent cohesion could be obtained in simulation, in which both of them were acquired on high levels of MC (Fig. 4). By increasing MC of wheat grains, the variation of obtained result of simulation corresponding to φ, by nonlinear elastic model was increasing like linear model one. But in the first three level of MC in the nonlinear predictions, the greater values than published values were observed and therefore the simulation diagram were as steep as experimental one between 15 and 17.5% of MC, but the goodness of fitting with experimental values is significantly smaller than linear model and was equal to 0.58. However in the high levels of MC there is more chance for nonlinear rather than linear model to predict φ values, as shown in Table 8.

Cohesion: The linear model only at first level of MC could predict the published C value in the acceptable area (Fig. 4). The fluctuation of published C values by increasing MC of wheat grains makes it hard to have a good fitness between simulation result and corresponding published values, as the simulation values of C had an increasing change of process that didn't report in literature. The relative low coefficient of correlation for predicting C by linear models had proved it (Table 8). But the simulation C values have been predicted in first, second and fourth levels of MC, had nearby values to its corresponding experimental values. This subject can be seen in the

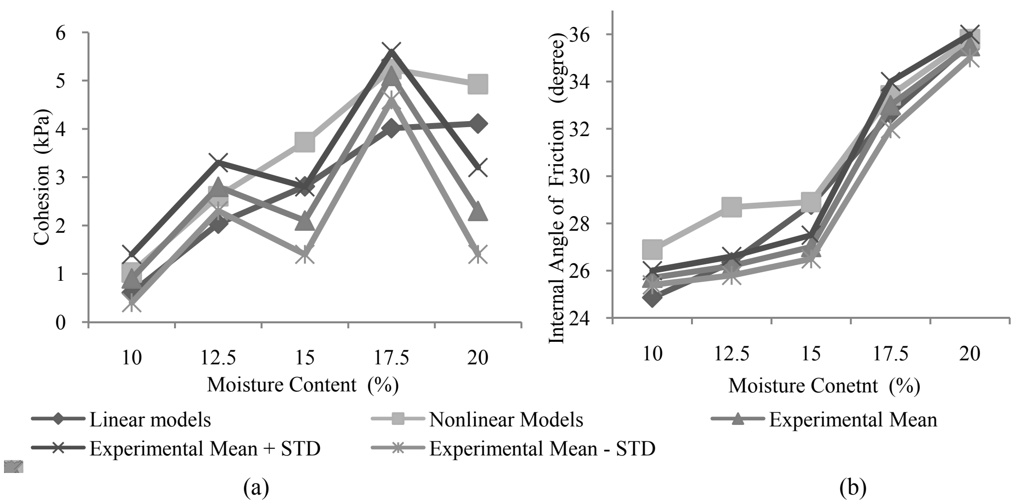


Fig. 4: Variation of strength properties of wheat grains with moisture content, Experimental and simulation results, (a) cohesion variation with MC, (b) internal angle of friction variation with MC

Table 8: Simulation results of strength properties, comparison with respective experimental values

		Contact model			
		Frictional linear elastic		Frictional Nonlinear Elastic	
Moisture content	Published data (S.D.)	Simulation data (S.D.)	Probability level (%)*	Simulation data (S.D.)	Probability level (%)*
Internal angle of friction		Correlation 0.98		Correlation 0.5	
10.0	25.7 (0.30)	24.860 (0.206)	90.77	26.890 (0.764	63.69
12.5	26.2 (0.40)	26.350 (0.073)	73.68	28.688 (2.036)	54.38
15.0	27.0 (0.50)	28.788 (0.328)	94.51	28.901 (1.875)	47.36
17.5	33.0 (1.00)	32.637 (0.425)	41.26	33.420 (0.123)	87.54
20.0	35.5 (0.50)	35.611 (0.126)	42.33	35.800 (0.107)	82.98
Cohesion		Correlation 0.70		Correlation 0.50	
10.0	0.9 (0.50)	0.608 (0.116)	80.04	1.026 (0.031)	90.71
12.5	2.8 (0.50)	2.037 (0.308)	79.58	2.604 (0.126)	63.64
15.0	2.1 (0.70)	2.809 (0.327)	75.46	3.725 (0.683)	78.37
17.5	5.1 (0.50)	4.012 (1.426)	37.51	5.237 (0.049)	82.91
20.0	2.3 (0.90)	4.109 (1.367)	57.45	4.925 (1.993)	57.26

data of prediction probability in low level of Mc, which has been shown in Table 8. The lowest chance of C values prediction was in the 17.5% of MC by linear model and equals to 37.51% and at the first level of MC the best prediction probability was observed which equal to 80.08% (Table 8).

The nonlinear model had a better success than linear model at all and could give a acceptable predictions of C in the first three levels of MC, but this model couldn't be able to represent the fluctuation path of C values by increasing MC of wheat grains and even showed a worse fitness with experimental published data by a correlation coefficient of 0.49. The considerable note in comparison of linear and nonlinear model to predicting C values was the greater values correspond to nonlinear models rather than linear ones at all of MC of wheat grains. It should be pointed out that the nonlinear models gave very acceptable probability levels in predicting C values at different MC levels. The best probability level was observed at first MC level, equal to 90.71% and the lowest chance was relevant to the last MC level and equals to 57%.

CONCLUSION

It has been proved in the present study that the DEM is able to capture the variation of bulk properties of wheat grains with MC of grains. At the same time, it must be noted that the simulation of bulk behavior of bio materials is strongly affected by the inter grain interaction and the shape of grains in modeling. Altogether the linear models have more capability in representing the form of strength Properties variation with Mc of grains rather than nonlinear ones. However on the average both of linear and nonlinear models have equal chance in correct predicting of strength properties of wheat assembly. Spherical grain models best simulated wheat grains in bulk properties tests. Boac *et al.* (2010) confirmed this claim in a similar study on soybean grains. In the other point of view, the φ has the same chance with C, to be predicted by presented DEM model in this study and this chance is about 70%. However the fitness of φ in different levels of MC is better than C, in simulation. This suggests that the modeling is a useful tool in the study of mechanical behavior of wheat and other cereal grains during storage processes as well as provision of data necessary in the design of appropriate machinery for the future modeling.

Appendix

The equation for the correlation coefficient is:

$$Correlation(X,Y) = \frac{\sum(x-\bar{x})(y-\bar{y})}{\sqrt{\sum(x-\bar{x})^2 \sum(y-\bar{y})^2}} \qquad (9)$$

where, $\bar{x}$ and $\bar{y}$ are the means values of two set of data.

Sokal and Rohlf (1995) proposed the equation 9 to calculate the t value, when the comparison of two mean values of two set of data must be considered (Sokal and Rohlf, 1995):

$$t = \frac{Population\ Mean - Sample\ Mean}{Standard\ Deviation\ of\ Sample \times \sqrt{\frac{n+1}{n}}} \qquad (10)$$

where, n is the number of sample data, and the degree of freedom is equal to $n-1$.

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