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Moisture-dependent physical properties of rapeseed – experimental and DEM modeling

J. Wiącek and M. Molenda*

Institute of Agrophysics, Polish Academy of Sciences, Doświadczalna 4, 20-290 Lublin, Poland

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Abstract. A series of tests were conducted to study the influence of moisture content of rapeseed on the physical properties of grain bedding. The load response of a grain assembly poured into a cubical test chamber and subjected to uniaxial confined compression was studied. Tests were conducted for the rapeseed of moisture contents of 7.5, 9, and 12%. It was determined that the load distribution varied considerably with the moisture content of the seeds. The lowest effective elastic modulus was obtained for a grain assembly composed of rapeseeds at moisture content of 12%. Comparison between experimental data and numerical modeling using the discrete element method (DEM) showed both, quantitative and qualitative agreement.

Keywords: moisture content, grain bedding, uniaxial confined compression, discrete element method

INTRODUCTION

The large-scale application and processing of granular plant materials in agriculture and many branches of industry, *eg* cosmetic, pharmaceutical or food industry, requires improved insight into the complex nature of grain and seed assemblies. Particular attention should be paid to the dependence of the mechanical behaviour of biological materials on internal storage and processing conditions, *eg* temperature, moisture content in air. These parameters have a significant effect on the properties of individual grains, which in turn have a significant effect on a grain assembly and the processes associated with granular systems. Particle moisture content affects both, geometrical and mechanical properties of grain and seed. Izli *et al*. (2009) showed that an increase in moisture content of rapeseed resulted in a linear increase in the axial dimensions, geometric mean diameter and sphericity of the seeds. The study on soybean and lentil seed at various moisture contents by Davies and El-Okene (2009) and Bagherpour *et al*. (2010), respectively, showed a similar relationship between the geometrical and physical properties of grains and their moisture content. The analysis of the lentil rupture forces showed that a greater energy was required to rupture grains at a lower moisture content than at a higher moisture content. An increase in the surface area of soybeans from 34 to 48 mm^2 was observed when the moisture content of soybean increased from 9.5 to 49.7%. In a study conducted by Horabik and Molenda (1989), on the relationship between the contact area of single grains of wheat on a smooth surface, a twofold increase in contact area was observed for an increase in moisture content from 8 to 18%. This increase was believed to be caused by the change in friction conditions at the surface of seed. The static coefficient of friction against surface increases as the moisture content increases (Davies and El-Okene, 2009; Izli *et al.,* 2009). The moisture content of biological materials oftentimes determines highly their elasticity. The modulus of elasticity and Poisson's ratio of grain bedding are the lowest for seeds at a higher moisture content (Molenda and Horabik, 2005). The deformation of a single grain may be classified as either elastic, viscoelastic or plastic based on its moisture content. Wojtkowski *et al*. (2010) showed that different contact models should be used to model the impact of grain of various moisture content against a flat surface. The experimental impact testing showed that the contact time was approximately twice as long for seeds with a moisture content of 34.2% compared with seeds with a moisture content of 5.5%. The authors determined that an elastoplastic model was effective in modeling the force-time relationship behaviour of dry rapeseed, whereas a viscoelastic model gave closer estimates of experimental force-time relationships for wet seeds.

The mechanical properties of a single kernel of grain oftentimes determines the effects observed in the grain assembly and the technological processes which the biological materials are subjected to. Molenda *et al*. (1995) determined

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*Corresponding author's e-mail: jwiacek@ipan.lublin.pl that in a study on wheat grain bedding a nonlinear relationship existed between the angle of internal friction in the assembly and the moisture content of wheat grain over a wide range of moisture contents. Izli *et al*. (2009) determined that the bulk density of rapeseed bedding decreases as the moisture content increases. Molenda and Horabik (2005) determined that for an increase in moisture content, the friction force and cohesion between grains increased resulting in a decrease in vertical pressure transmitted in the lateral direction. Therefore, the pressure ratio, defined as the ratio of lateral to vertical pressure decreases as the moisture content of the grain assembly increases. Horabik and Rusinek (2002) determined that during uniaxial compression tests the largest decrease in pressure ratio occurred within rapeseed bedding for tests conducted with wheat, barley, corn oats and rapeseed. The study conducted by Blight (1995) on the effect of moisture on properties of barley and rice grains stored in silos showed that compressibility, shear stress, angle of internal friction and lateral pressure ratio determined for barley increase as a moisture content increases. For the rice, the increase in moisture content resulted in increase in compressibility of grains. The shear stress, angle of internal friction and lateral pressure ratio increased with moisture content increasing from 0 to 10%. The further increase in moisture content of rice grains to 15% resulted in decrease in value of parameters.

Experimental and analytical research methods have been used for many years to investigate and predict phenomena occurring in grain assemblies. The difficulties in relating the properties of single kernels of grain to those in bulk have resulted in development of computational techniques which are useful for a more detailed analysis of the behaviour of grains. One of the most popular methods of computer modeling, which takes into account the discrete nature of granular material is the discrete element method (DEM) (Cundall and Strack, 1979). The discrete element method allows for a detailed analysis of the interactions between single objects in grain bedding which ultimately determine the mechanical properties of the whole assembly. While this method is commonly used to model processes in granular materials of mineral origins, it is infrequently applied to agricultural granular materials in bulk. The main reason for this is that there exists a lack of knowledge of the contact forces, and how to model these forces, in biological materials. Tijskens *et al*. (2003) showed the need to undertake research to link mechanical properties of biological materials to contact force models. The experimental and numerical study conducted by Chung and Ooi (2005) on the uniaxial compression testing of corn grains in a cylindrical container showed that the DEM prediction is in excellent agreement with the results of this type experiment. They determined that the Hertz-Mindlin no-slip contact model is capable of producing quantitative predictions for corn grains even though the representation of the actual grain shape was not very accurate.

The mechanical behaviour of a rapeseed assembly was studied to determine the influence which moisture content plays in the uniaxial compression of biological materials.

The discrete element method was then used to model the experimental data collected during these tests to determine how well this modeling tool can be applied to the modeling of agricultural materials in bulk.

The comparison between physical and numerical results obtained through application of discrete element method was conducted which make possible to pave the way for adoption of the DEM computational technique for agricultural materials.

MATERIALS AND METHODS

Laboratory tests were conducted in this study using a uniaxial compression apparatus. The uniaxial confined compression test is a common test method used to determine mechanical properties of granular materials. Uniaxial compression test allows one to analyze the stress-strain characteristics of granular solid and to determine material parameters such as lateral-to-vertical pressure ratio, k, Poisson's ratio, v, or effective elastic modulus, E. The effective elastic modulus, E, is defined as (Eurocode 1, 2006):

$$E = H\frac{\Delta\sigma_z}{\Delta v}\left(1 - \frac{2k_L^2}{1+k_L}\right),$$

where: H is a initial length of sample, $\Delta\sigma_z$ – the change in vertical pressure, Δv – change in vertical displacement, k_L – a ratio of the change in lateral pressure to change in vertical pressure.

The results of these tests are often used by technological process designers. Both, physical (Rusinek *et al*., 2007; Sawicki, 1994) and numerical (Azadi *et al*., 2008) modeling of granular solids loaded in compression of granular solid can provide valuable knowledge necessary for efficient design and useful scientific insight.

Eurocode 1 (2006) recommends that for granular particles a cylindrical testing device be used to measure the lateral pressure ratio, k, the ratio of horizontal stress to vertical stress. The device must have a diameter, D, of at least 5 times the size of the largest particle but not larger than 10 times the size of the largest particle and the device must have has a minimum height of at least 0.3 to 0.4 D. The Eurocode, as well as majority of published analyses consider the cylindrical sample to be loaded under axi-symmetrical stress with the assumption that the material is isotopic. Numerous studies have shown that granular materials are anisotropic and that their properties are dependent on both the shapes of particles and method of generation of the bedding (Oda, 1978; Molenda *et al*., 1996). Therefore for this study an apparatus with a rectangular cross section (Fig. 1) was constructed to measure loads in both the horizontal and vertical directions as the sample undergoes deformation in the vertical direction. The tester was machined from galvanized

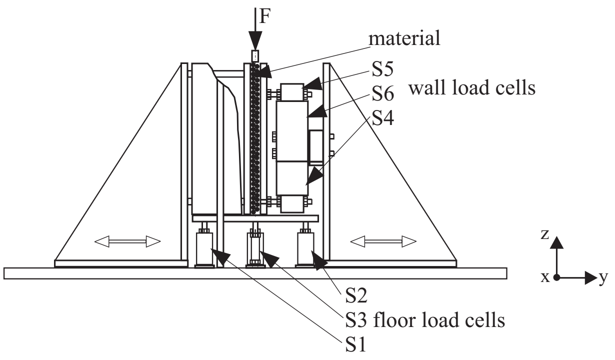

Fig. 1. Schematic of uniaxial compression apparatus used for testing seeds (Rusinek *et al.*, 2007).

steel with a thickness of 6 mm, giving an essentially rigid boundary under the loading applied. The tester had a rectangular cross-section 21 mm wide by 120 mm long and was 120 mm tall. The two 120 mm high boundary walls of the apparatus, were attached to the solid support plate at the distance of 120 mm. The base of apparatus was supported on three load cells (S1, S2 and S3) to measure vertical loads. The two adjustable walls of the apparatus (perpendicular to the plane of the figure) were placed at a distance of 21 mm from each other and were located 1 mm above the floor to avoid load transmission onto the floor. The vertical and horizontal stresses were measured by means of load cells fixed to the apparatus wall and bottom platen. The right hand side wall of apparatus (Fig. 1) was supported on three load cells (S4, S5 and S6) to measure normal wall load. The normal load exerted on the top platen was measured with load cell (S0). The apparatus was placed on the table of a testing machine under its crosshead. The specimen was loaded from the top platen with a displacement speed of 0.35 mm min^{-1}. After the normal lid pressure reached a reference value of 100 kPa, the top platen was stopped and unloaded with the same speed.

The confined uniaxial compression tests were conducted for rapeseed (Licosmos variety) at moisture contents of 7.5, 9, and 12%. The seeds were poured into the test chamber (21 mm thick, 120 mm wide and 120 mm high) and then leveled. The chamber was filled using an eccentric filling technique with the eccentric filling stream of grain located against a side wall. Three replications were performed for each moisture content and average values are presented further in the article.

In this study, numerical simulations were conducted using the discrete element method (DEM). Discrete element method provides opportunity for more detailed investigation of granular systems due to its microstructural approach (Cundall and Strack, 1979) and the potential for modeling 2D and 3D processes in granular solids composed of particles of various shapes. In this modeling technique after contacts between particles in system are detected, contact forces at each incremental time step are calculated. The time step is expected to be small enough to allow one to assume a constancy of translational and rotational accelerations. Integration of equations of motion for each particle provides velocities and positions of particles.

In this study a non-linear Hertz-Mindlin no-slip contact model (Ji and Shen, 2004) was applied using an with elastic spring and viscous damper model in the normal direction (Fig. 2a) and spring, damper and slider model in the tangential direction (Fig. 2b). Spring models assume an accumulation of energy in system, whilst damper and slider models assume energy dispersion. The tangential contact force is limited by the Coulomb friction law which assumes that particles slide over each other when the tangential force is higher than friction force.

Three-dimensional DEM simulations were conducted using EDEM software. In this simulation model uniform 1.9 mm diameter spheres with mechanical parameters of rapeseed were assumed to be poured into a steel chamber of rectangular cross-section (Fig. 3). Particles randomly generated in the whole volume of box settled down onto the bottom of box under gravitational forces. The top lid of box was then assumed to move down with constant velocity until the normal lid pressure reached 100 kPa. Unloading was modeled assuming the lid moved upwards until there was no contact between specimen and platen. The initial model simulating the compression test was composed of 49 000 grains and required a large amount of computational time and power. To reduce the required computational requirements a series of numerical test were conducted to determine a representative elementary volume, which is the smallest specimen over which a measurement can be made that will yield a value representative of the large volume (bedding). It was determined that a representative elementary volume 10.5 mm thick, 60 mm wide and 60 mm high filled with 5 500 grains was able to accurately model the test conditions. Additional simulations were carried out using the representative elementary volume for compression tests conducted at rapeseed moisture contents of 7.5, 9, and 12% assuming a loading rate of 0.05 m s^{-1} (3 000 mm min^{-1}). The load rate, higher than the one suggested by Eurocode 1 (2006), decreases computational time while asserting the stability of the system (Wiącek, 2008). For each condition three replications were performed for grain assemblies composed of 5500 rapeseed at various moisture contents.

Experimentally established input parameters for rapeseeds at various moisture contents (Wiącek, 2008) and mechanical parameters for steel (eFunda) are listed in Table 1.

RESULTS AND DISCUSSION

The evolution of modulus E with vertical pressure for grain assemblies at moisture contents of 7.5, 9, and 12% during the loading stage is shown in Fig. 4. The results are

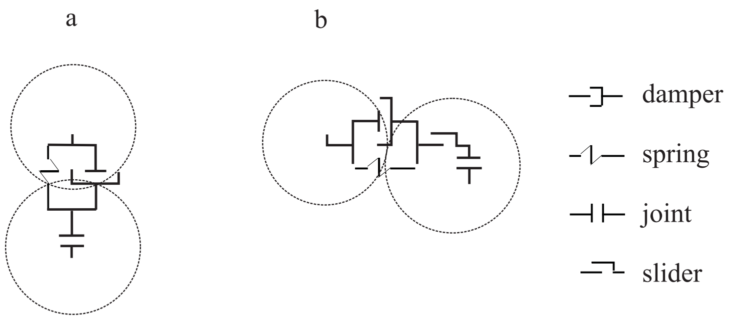

Fig. 2. Contact mechanics models: a – viscous - elastic in normal direction, b – viscous - elasto - frictional in tangential direction.

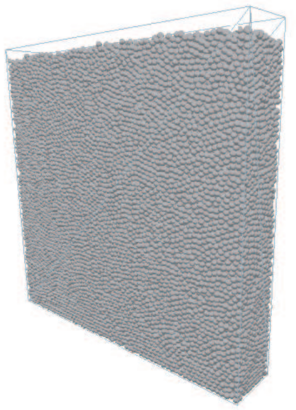

Fig. 3. Initial configuration of numerical specimens composed of 49 000 rapeseed.

plotted using the mean values for three simulations, with the error bar indicating ± one standard deviation. The average porosity of experimental samples was determined to be 0.275. For a given moisture content, the modulus *E* was found to increase slowly for an increase in vertical pressure. An increase in rapeseed moisture content resulted in a decrease in the effective elastic modulus of grain bedding as a consequence of a decrease in the stiffness of the kernel endosperm. An increase in moisture content of rapeseed from 7.5 to 9% resulted in only a slight change in the elasticity of grain assembly as compared to the change resulting from an increase in moisture content from 9 to 12%.

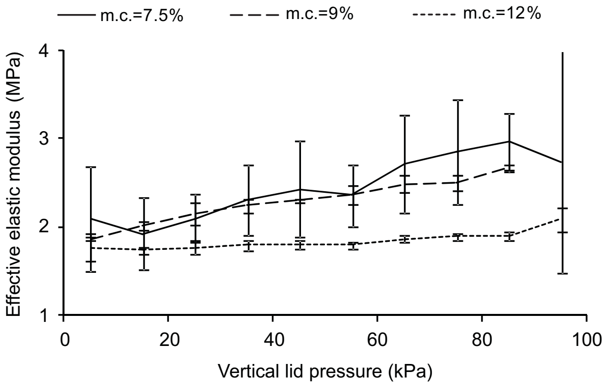

Fig. 4. Effective elastic modulus – vertical lid pressure relationships for grain bedding at various moisture contents (m.c.).

Table 1. DEM input parameters (eFunda; Wiącek, 2008)

Parameter, unit	Rapeseed			Steel
	Moisture content (%)			
	7.5	9	12	
Poisson's ratio	0.24	0.17	0.16	0.3
Shear modulus (MPa)	159	99	75	200 000
Coefficient of static friction	rapeseed-rapeseed 0.234	rapeseed-rapeseed 0.379	rapeseed-rapeseed 0.447	rapeseed-steel 0.43
Coefficient of rolling friction		rapeseed-rapeseed 0.01		rapeseed-steel 0.01
Coefficient of restitution		rapeseed-rapeseed 0.4		rapeseed-steel 0.4
Density (kg m^{-3})		1 050		7 800

Figure 5 shows pressure ratios for the three different levels of rapeseed moisture contents during the loading and unloading stages of compression test. The standard deviation bars are also indicated in the figures.

The highest pressure ratios were obtained for grain bedding at the lowest moisture content during both, loading and unloading. At 50 kPa, an increase in moisture content from 7.5 to 9% resulted in a 17% decrease in pressure ratio at load pressure of 50 kPa. A further increase in rapeseed moisture content to 12% at the same pressure resulted in an additional 10% decrease in lateral-to-vertical pressure ratio. As the moisture content increases the friction force and the cohesion between grains increase resulting in a smaller part of the vertical load being transmitted in the lateral direction. Consequently, the pressure ratio decreases as the moisture content of seeds increases.

The relationships between the effective elastic modulus and vertical lid pressure for numerical rapeseed assemblies composed of 49 000 and 5 500 grains are presented in Fig. 6. The stiffness of the more numerous grain bedding is slightly higher than that of the simplified model comprised of 5500 grain. This is believed to be caused by the differences in porosity assumed within each model. Comparison between pressure ratios calculated for both numerical rapeseed beddings (Fig. 7) shows that DEM predicts almost identical pressure distributions in specimens composed of various number of grains. These results suggest that the simulation model containing the more numerous assembly may be replaced by the less numerous one to model uniaxial compression test of rapeseed bedding. This would save computational time without losing accuracy of simulation.

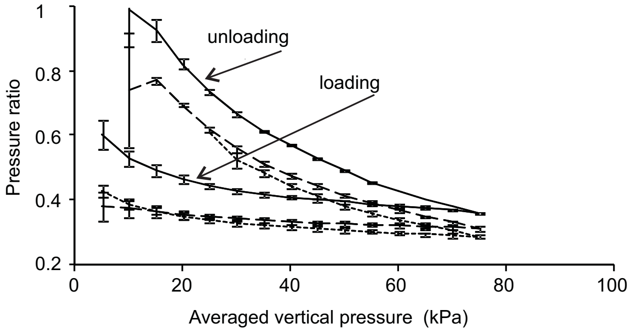

Fig. 5. Lateral-to-vertical pressure ratio – vertical pressure relationship for grain bedding at various moisture contents (m.c.). (Explanations as in Fig. 4).

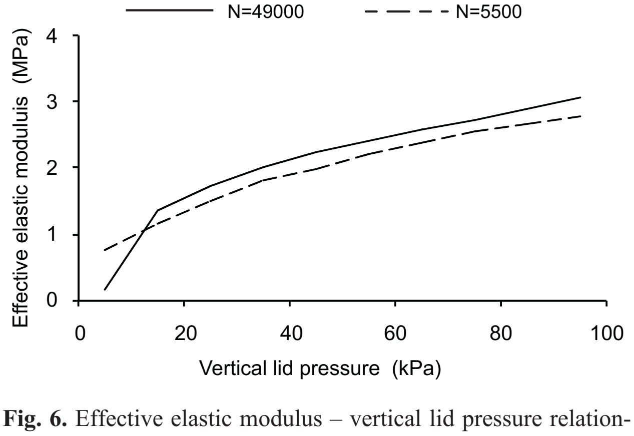

Fig. 6. Effective elastic modulus – vertical lid pressure relationships for numerical grain beddings composed of 49 000 and 5 500 grains at moisture content of 9%.

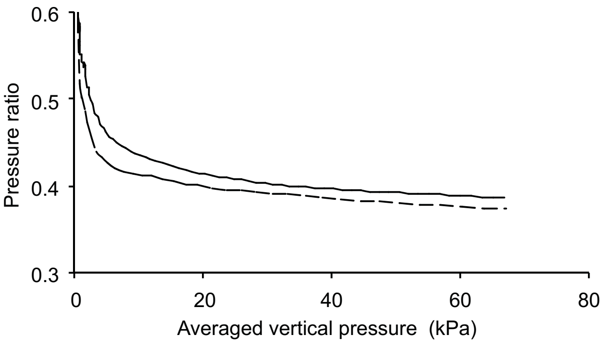

Fig. 7. Lateral-to-vertical pressure ratio – vertical pressure relationship for numerical grain beddings composed of 49 000 and 5 500 grains at moisture content of 9% (Explanations as in Fig. 6).

The comparison of the DEM predictions of effective elastic moduli and pressure ratios for rapeseed beddings at various moisture contents are compared with experimental results are shown in Figs 8-10. The results are plotted using the mean values with the error bars indicating ± one standard deviation.

As shown in Fig. 8, the DEM simulations predicted lower effective elastic modulus than that measured in these experiments for each level of rapeseed moisture content. These differences may be attributed to a number of factors including the number of grains in the physical tests compared to that used in the numerical rapeseed assemblies, the non-spherical shapes of real rapeseed and the looser initial packing (higher porosity) of the numerical simulation compared to that of the test samples. Perfect spheres of the same size rotate more easily than in a real system where a variation in the natural grain size exists, actual kernels have a non-perfect shape and a variability in surface friction from one particle to another. These difference can also be a result of imperfections in the test apparatus including among others: limited accuracy of its dimensions, non perfectly rigid walls and their supports, imperfect plane surfaces or uneven distribution of frictional properties. The effective elastic modulus of physical and numerical rapeseed bedding increases as a vertical lid pressure increases, however the higher increase in stiffness for numerical specimens was observed. The differences between modulus E of numerical and experimental samples decrease as a rapeseed moisture content increases.

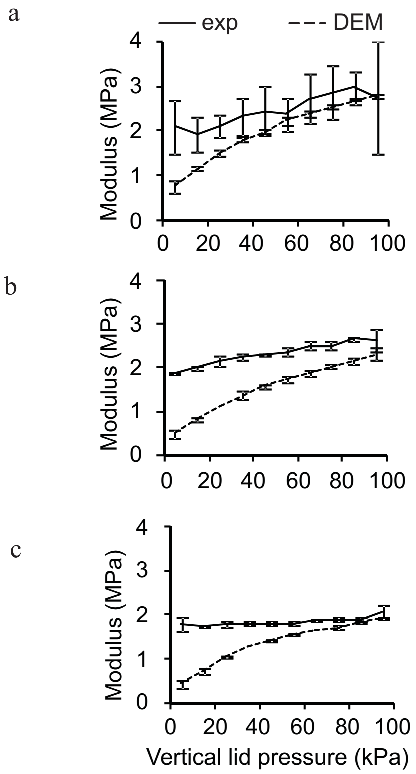

Fig. 8. Effective elastic modulus – vertical lid pressure relationships for experimental and numerical samples at various rapeseed moisture contents: a – 7.5, b – 9, c – 12%.

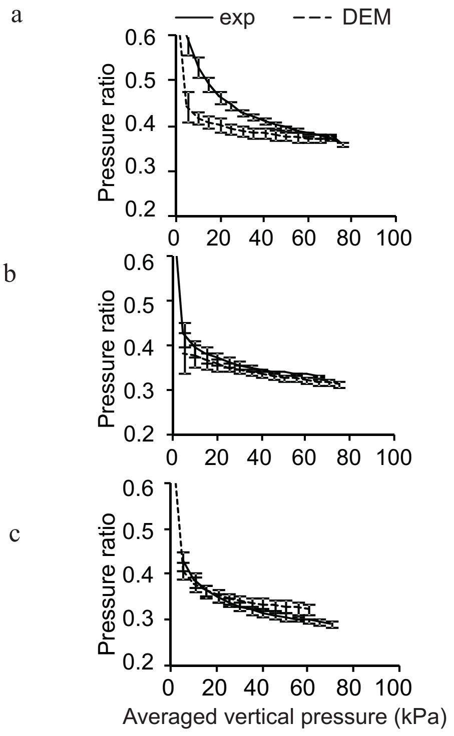

Fig. 9. Lateral-to-vertical pressure ratio – vertical pressure relationship for experimental and numerical samples at various rapeseed moisture contents: a – 7.5, b – 9, c – 12%.

The comparison between the effective elastic modulus - vertical pressure relationships for physical and numerical samples at various rapeseed moisture contents shows qualitative agreement between experimental and DEM results. In both cases (experimental and DEM modeling) the stiffness in the rapeseed bedding was observed to increase with an increase in vertical lid pressure. At vertical pressures less than 50 kPa DEM modeling predicted an effective elastic modulus significantly smaller than those observed during experimental testing. At vertical pressures above 50 kPa DEM modeling agreed well for moisture contents at 7.5 and 12%.

Both, qualitative and quantitative agreement between experimental and numerical relationships between pressure ratio and vertical pressure was found for each level of rapeseed moisture content during the loading stage of compression test (Fig. 9). DEM predicted lower pressure ratios for rapeseed moisture content 7.5% at vertical pressure lower than 50 kPa. The pressure ratio decreased as the grain moisture content increased. In both, experimental and numerical tests slight differences between pressure ratios calculated for 9 and 12% moisture contents was obtained. It was probably due to approximate fabric of these grain beddings, the same porosities and coordination numbers in numerical specimens.

The results of these study indicate that the mechanical response of a granular assembly subjected to uniaxial compression is significantly affected by moisture content of grains. Both, DEM numerical modeling and experimental tests revealed differences in the elasticity and the stress transmission within rapeseed assemblies at various grain moisture contents. The findings show that the discrete element method is a useful tool in to predicting the mechanical behaviour of grain assemblies and may be successfully applied to agricultural products For the case presented in this paper, it was proven that this technique can be used to accurately model both, qualitative and quantitative comparison between experimental and numerical results.

CONCLUSIONS

1. The effective elastic moduli of both, numerical and experimental assemblies were affected by rapeseed moisture content.

2. The lateral force transmission in a confined granular system considered as the ratio of horizontal to vertical pressure is sensitive to moisture content of sample when moisture content is lower than 9%.

3. A good qualitative agreement between effective elastic modulus – vertical lid pressure relationships calculated from numerical and physical results was obtained for granular specimens at various moisture contents.

4. DEM predicted a softer response for the spherical assembly as compared to the experiments on rapeseed.

5. A good quantitative and qualitative agreement between pressure ratio – vertical pressure relationships calculated from numerical and physical results was obtained for granular specimens at various moisture contents.

6. The high capability of discrete element method to predict mechanical behaviour of granular materials of biological origin was confirmed.

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