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DISCRETE ELEMENT METHOD (DEM) AS A TOOL FOR INVESTIGATING PROPERTIES OF GRANULAR MATERIALS

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Key words: granular materials, numerical methods, Discrete Element Method (DEM)

With an increase in the scale of industrial operations the necessity of understanding the behaviour of granular materials and examining their properties becomes increasingly important. It is associated with rapid development of industries such as: food, chemical, pharmaceutical, cosmetic *etc*., in which materials in granular form are processed. One way of description of macroscopic behaviour of granular systems is a model including interactions between individual particles and between particle and elements of construction. Current needs of both technology and science call for the new research methods that provide more accurate results and enable closer examination of processes. Development of computational techniques resulted in the elaboration of Discrete Element Method (DEM).

This article is focused on DEM as proposed by Cundall & Strack [1979] which enables interpretation of processes occurring in granular bedding considering phenomena on interparticle scale. The limitations and capabilities of DEM as well as results of modelling experimental investigations are addressed.

INTRODUCTION

Specific and to a large extent still unknown properties of granular materials have recently attracted growing interest of science and technology. The wide use of these materials in the food industry results in the following classification of granular materials based on applied processes: ground powders (*e.g.* sugar, spices), spray dried (*e.g.* milk, egg), drum-dried (*e.g.* mashed potatoes, lactose), agglomerated powder (*e.g.* coffee, instant milk), precipitated powder (*e.g.* protein isolate), crystalline powder (*e.g.* salt, sugar) and a mixture of powders (*e.g.* dry fruit drink). Granular materials are often considered as the fourth state of matter [Jaeger *et al*., 1996] with properties of solids, liquids and gases. The wide industrial use of particulate materials and lack of full understanding of numerous processes occurring in beddings encourage investigations of that media. Numerous studies were aimed at deriving in-bulk material properties from interparticle interactions and the question still remains of large interest [Mühlhaus & Vardoulakis, 1987; Langston *et al*., 1997; Yang & Hsiau, 2001]. Investigations of granular systems of large scale brought about many questions that have not been answered till now. Throughout over hundred years of investigations of particular materials experimental, analytical and numerical methods have been elaborated.

This paper is focused on the application of Discrete Element Method being a common computational method for studying properties of granular assemblies. Even though this numerical technique is very useful, a lot of difficulties emerge when performing DEM simulations. One of essential questions are: establishing a simulation time step and selection of model for contact force and time scheme. This article presents two-dimensional simulations: of popular laboratory technique – direct shear test, and of practical effect – process of silos discharge. Computational model, limitations and capacities of applied method are presented as well.

MATERIALS AND METHODS

Discrete Element Method (DEM). A lack of understanding a relationship between behaviour of granular media and that of particular grains called for new research methods. A decrease in prices of computers made numerical methods a common and efficient tool for examining mechanics of granular materials. One of them has been Discrete Element Method proposed by Cundall and Strack in 1979 [Cundall & Strack, 1979]. This was the first method that enabled simulation of behaviour of relatively large assembly of particles (>1000). Originally, these authors proposed algorithm for two-dimensional simulations, but recently efficient programs for three-dimensional simulations have been elaborated [Langston *et al*., 1997; Landry *et al*., 2004]. The majority of available codes enable modelling with the geometrically simplest elements, such as discs and spheres, albeit examinations of systems of grains of more complex shape are possible as well [Cleary & Sawley, 2002; Langston *et al*., 2004].

Discrete element method treats bulk solid as a system of distinct interacting bodies. Each particle is identified sepa-

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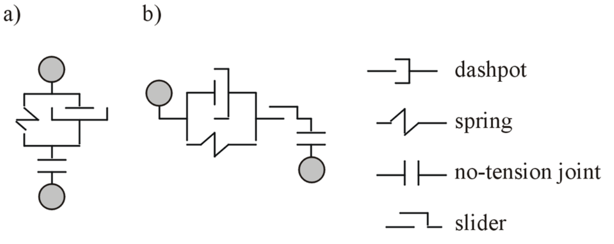

FIGURE 1. Contact model for DEM simulations in the normal (a) and tangential (b) directions.

rately having its own mass, velocity and contact properties. Contacts between cylindrical elements in the system are modelled by the set of linear springs, dashpots and joints in normal and tangential directions and frictional slider in tangential direction (Figure 1).

The contact force results from elastic, viscous and frictional resistance which can be modelled as the spring, dashpot and shear slider. The spring expresses elastic interaction while the dashpot models dissipation of energy in the system. Shear slider, that represents frictional force at contact point, starts its operation when the following inequality is met:

$$\left|F_t\right| \geq \mu F_n, \tag{1}$$

where: F_t and F_n are tangential and normal forces, respectively, and μ is a coefficient of friction.

Such a contact model allows calculation of forces acting on each particle. Position, velocity and acceleration of the particle are estimated by numerical integration of the Newton's second law:

$$m_i\ddot{\mathbf{x}}_i = m_i\boldsymbol{g} + \sum_j F_{ij} \qquad I_i\ddot{\boldsymbol{\theta}}_i = \sum_j (r_{ij} \cdot F_{ij}) \tag{2}$$

where: m_i is a mass of particle i, $\ddot{\mathbf{x}}_i$ is its translational acceleration, $\mathbf{g}$ is acceleration of the gravity, F_{ij} is the force at contact with neighbouring particles j, I_i is a moment of inertia, $\ddot{\boldsymbol{\theta}}_i$ is particle rotational acceleration, $\mathbf{r}_{ij}$ is the vector directed from the centre of the particle i to the contact point with particle j.

Deformations enforced by contacts between particles or particle and boundary during collision are represented by overlap at contact point. Two methods of modelling interaction of two particles during impact have been proposed. Hard-sphere model does not require as short simulation time step as soft-sphere model does as a result of different way of description of velocities and positions of elements in the two methods. Using hard-sphere model involves the loss of some data, which limits its applicability to dilute free-flowing systems [Di Renzo & Di Maio, 2005].

To enable application of DEM for more complex and time-consuming processes Iwashita & Oda [2000] improved algorithm of Cundall & Strack [1979]. Owing to its capacities DEM is nowadays an effective tool used for modelling numerous processes occurring in granular systems, such as: particles segregation [Sakaguchi *et al*., 1998], particles flow [Langston *et al*., 1997, 2004], silos discharge [Yang & Hsiau, 2001; Sakaguchi *et al*., 1994; Masson & Martinez, 2000], shear behavior [Iwashita & Oda, 2000; Sakaguchi & Favier, 2000], *etc*.

Determination of simulation time step. Calculation of a simulation time step is one of essential questions in DE modelling. Sufficiently short time step ensures stability of the system and enables stimulation of the real processes.

According to Timoshenko & Goodier [1970] and Johnson [2004], during motion of particles in a granular system the disturbances propagate in a form of Rayleigh waves along surface of solid. The simulation time step is a part of Rayleigh time which is taken by energy wave to transverse the smallest element in the particular system. It should be so short that disturbance of particle's motion propagates only to the nearest neighbours. It is assumed that velocity and acceleration are constant during the time step. The time step should be smaller than critical time increment calculated from theory. A number of equations have been proposed for calculation of a critical time step [Cundall & Strack, 1979; O'Sullivan & Bray, 2004], however usually it is estimated based on natural frequency in a linear spring system [Raji & Favier, 2004]:

$$\Delta t_c = f\sqrt{m_i / k}, \tag{3}$$

where: k is effective stiffness and f is a factor. The choice of proper value of the constant f is very important but not easy. The reason of difficulties is a fact that the f depends strongly on packing configuration, number of contacts and properties of particles. It is different for two- and three-dimensional simulations as well [O'Sullivan & Bray, 2004].

Models of contact interaction. Application of a proper contact model within DEM simulations enables accurate description of particles collision. The particle contact forces occur only when particles penetrate or overlap. For circular particles the overlap occurs when:

$$\Delta_{ij} = (r_j - r_i) - |\mathbf{x}_j - \mathbf{x}_i| \geq 0, \tag{4}$$

where: Δ_{ij} is the amount of overlap between particles i and j, r is a particle radius and $\mathbf{x}$ is the position vector for the particle centre. Linear and non-linear contact models may be applied. In the former model normal contact force is a linear function of the overlap Δ_{ij} and relative velocity of particles $\dot{\Delta}_{ij}$:

$$F_{ij} = k\Delta_{ij} + c\dot{\Delta}_{ij} \tag{5}$$

where: k is coefficient of stiffness and c is coefficient of damping. The linear model is sufficient to investigate simple processes occurring in grain assembly for elastic collisions. In certain cases, in spite of its simplicity linear contact model provides results close to experimental data [Di Maio & Di Renzo, 2004]. The more complex processes should be examined by application of non-linear contact model that was proposed by Hertz [1882] for normal direction:

$$F_{ij} = k\Delta_{ij}^{\alpha} + c\Delta_{ij}^{\beta}\dot{\Delta}_{ij} \tag{6}$$

where: α and β are the index, and by Mindlin [1949] for tangential direction. These models pose Hertz-Mindlin contact theory for elastic granular materials. The need of examining materials with various properties enforced extending the

Hertz-Mindlin theory for plastic and non-elastic interactions of particles. Depending on material properties and simulation conditions values of α of 3/2 and β of 1/2, 1/4 or 3/2 have been proposed for the constants [Ji & Shen, 2004].

Two time integration algorithms can be applied. In the case of linear model explicit time integration scheme is recommended where equation of motion of each particle is integrated independently on other elements for each time step. Contacts with neighbouring grains are checked at the end of each time step. Modelling processes by application of non-linear contact model requires more exact and time-consuming impact time integration scheme [O'Sullivan & Bray, 2004].

Computational model. In the reported project two-dimensional simulations were carried out using Wassgren's software [Wassgren, 1997]. The normal contact model consisted of spring and dashpot elements while the tangential contact model included spring and sliding elements. Two processes direct shear test and discharge of silo were modelled. Simulations of direct shear test were performed for 500, 1000 and 2000 circular elements having diameters of 1.5±0.15 mm and density of 2500 kg/m^3 and filling shear box of dimensions of 20 x 50 mm, 30 x 70 mm and 40 x 100 mm, respectively. Different values of friction coefficient (μ=0.1, 0.3, 0.5) and simulation time step ($\Delta t=1\times10^{-5}$, 2.5×10^{-5}, 5×10^{-5} s) were chosen to examine their influence on the accuracy of the results obtained. In the first stage of simulation grains were generated and placed randomly in a shear box. Bedding was sheared under condition of vertical normal pressure of 20 kPa applied to the top cover which was allowed to rotate around its axis of symmetry (Figure 2). Direct shearing was modelled by moving lower part of the box horizontally with velocity of 0.005 mm/s with maximum shear displacement of 10% of box length.

The second examined question within the reported project was an influence of friction on flow pattern during silo discharge. Simulations were carried out for 800 circular elements having an average diameter of 1 mm and friction coefficient between particle and the wall μ of 0.1 or 0.7. Coefficient of friction of grains was constant and equalled 0.1. Particles filled wedge-shaped hopper silo 20 mm in diameter (D) and 100 mm in height, hopper half angle φ was of 84° and orifice width D_o of 4 mm (Figure 3). Simulations were performed with a time step Δt of 5×10^{-5} s.

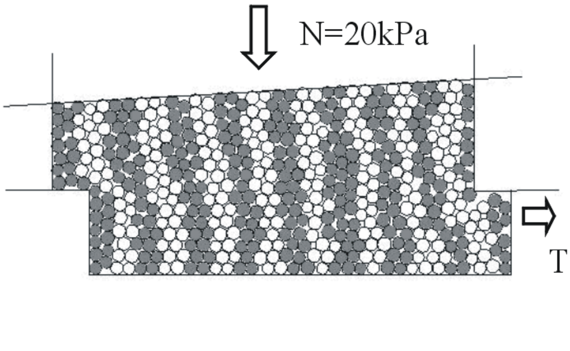

FIGURE 2. Direct shear box.

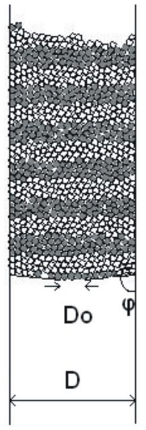

FIGURE 3. Model of the silo.

RESULTS AND DISCUSSION

Direct shear test

Simulations of direct shear test were carried out for different values of time steps. A ratio of shear (T) to normal (N) forces (Figure 2) was calculated from the shear box walls normal and tangent reaction forces [Thornton & Zhang, 2003]. The T/N ratio was analysed as the effective measure of frictional resistance of grain bedding during shearing. Simulations with time increments of 1×10^{-5} s and 2.5×10^{-5} s gave similar result. Increasing the simulation time step to 5×10^{-5} s brought about instability of the system and unacceptable results. Further investigations were done with $\Delta t=2.5\times10^{-5}$ s.

Models of Jenike's [1961] shear box filled with 500, 1000 or 2000 elements were used to examine the influence of a number of particles on behaviour of the bedding. The relationships between T/N values and displacement obtained in simulations for elements with friction coefficient of 0.1 are presented in Figure 4. With an increase in the number of particles in the system the amplitude of T/N ratio values oscillations decreased. This was probably a result of smoothing the course due to averaging the T/N values in larger systems.

Material parameters were found to influence essentially processes occurring in grain bedding. Changes in T/N values estimated for particles with various friction coefficients are

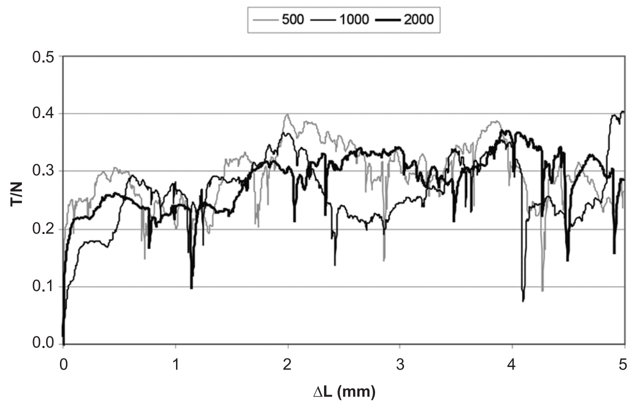

FIGURE 4. Evolution of T/N ratio *versus* displacement for different number of elements.

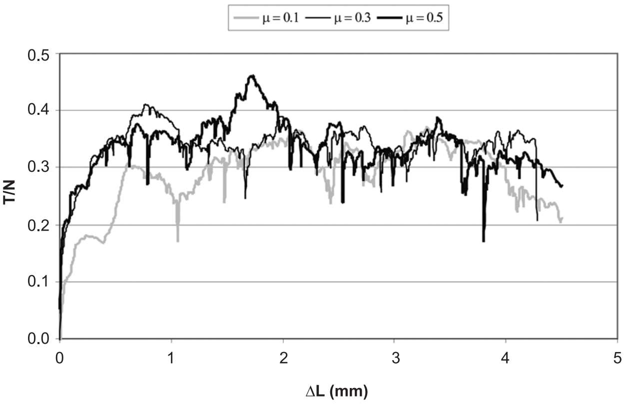

FIGURE 5. Evolution of T/N ratio *versus* displacement for different values of friction coefficient.

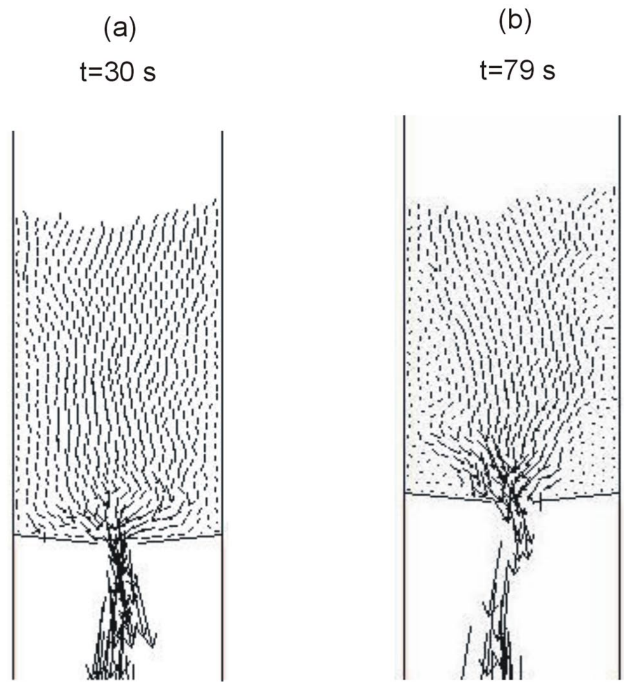

FIGURE 6. Distribution of velocities of particles for μ=0.1 (a) and μ=0.7 (b).

shown in Figure 5. The initial shear modulus was found to be influenced by the interparticle friction. During the steady flow, the T/N ratio stabilized at the value of approximately 0.35 irrespective of the grain-to-grain friction. This result suggests that during the steady flow the geometrical structure of the bedding plays a more important role in effective friction resistance of granular assembly than the grain friction. The T/N ratio calculated for μ=0.3 (the closest to the steady T/N ratio) was observed to change in a more smooth way than that computed for μ=0.1 or 0.5. A successive rotation of the top cover of the shear box following rearrangement of particles was observed during the shearing process (Figure 2).

Simulation of flow pattern

Examination of the accuracy of simulation code was performed also for modelling discharge of silo. Eight hundred particles were used having coefficients of friction of 0.1 or 0.7, in two simulation variants. Particles generated randomly fell down under gravity in wedge-shaped hopper silo and settled at the bottom. After completing the stage of filling the orifice, the discharge orifice was opened and discharge commenced. Depending on material properties of particles and the silo two types of flow patterns were observed: mass flow or funnel flow. The influence of the coefficient of friction between particle and wall on flow pattern was examined. In the case of μ=0.1 nearly uniform flow of material in the whole silo (mass flow) was observed (Figure 6a). Velocities of particles in the central part of hopper were found larger than those of particles located in closer distance to the wall. The difference was larger in the case of the coefficient of friction reaching 0.7 (Figure 6b). In the case of μ=0.7, large regions of stagnant material formed close to the wall and in the hopper of the silo that characterize funnel flow (Figure 6b).

CONCLUSIONS

The two-dimensional DEM simulations were carried out to model direct shear test and process of silo discharge giving reasonable results. Selection of the value of simulation time increment was found to be essential for stability of the system and quality of results. The analysis of evolution of ratio of tangential to normal forces acting on grain bedding while shearing showed a decrease in amplitude of oscillations of T/N values in larger systems. Coefficient of friction of grain strongly influenced behaviour of granular material. Depending on properties of particles different flow patterns developed during discharge of wedge-shaped hopper silo. The particles having lower friction coefficient discharged in a form of mass flow while funnel flow type was observed in the case of higher friction coefficients.

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METODA ELEMENTÓW DYSKRETNYCH (DEM) NARZĘDZIEM BADANIA WŁAŚCIWOŚCI MATERIAŁÓW SYPKICH

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Wzrost skali operacji przemysłowych wykonywanych na materiałach ziarnistych w wielu gałęziach przemysłu (spożywczego, chemicznego, farmaceutycznego, kosmetycznego i in.), niosie konieczność zrozumienia ich zachowania oraz badania ich właściwości mechanicznych. Jednym ze sposobów interpretacji efektów obserwowanych w ośrodkach granularnych jest stosowanie technik numerycznych do ich modelowania. Szerokie stosowanie materiałów w formie ziarnistej niesie potrzebę poszukiwania lepszych metod badawczych, których wykorzystanie zapewniałoby dokładność wyników oraz umożliwiało precyzyjną interpretację procesów zachodzących w złożu.

Rozwój technik komputerowych w drugiej połowie XX wieku zaowocował powstaniem Metody Elementów Dyskretnych (DEM).

Celem artykułu jest prezentacja, zaproponowanej przez Cundalla & Stracka [1979] metody numerycznej DEM, umożliwiającej analizę efektów obserwowanych w ośrodku sypkim poprzez uwzględnienie procesów zachodzących na poziomie mikrostrukturalnym. Zaprezentowano ograniczenia i możliwości metody oraz wyniki modelowania wybranych testów eksperymentalnych.