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CALIBRATION OF BULK MATERIAL MODEL IN DISCRETE ELEMENT METHOD ON EXAMPLE OF PERLITE D18-DN

KALIBRACJA MODELU MATERIAŁU SYPKIEGO W METODZIE ELEMENTÓW DYSKRETNYCH NA PRZYKŁADZIE PERLITU D18-DN

Analytical methods for calculations of the transport machinery are often insufficient especially when untypical granular materials are considered. Discrete Element Method (DEM) is a very useful numerical tool supporting designing and optimization of the transport equipment. However, to obtain reliable DEM simulation results an accurate set of input parameters values is needed. The most common calibration approach is to make use of a procedure where laboratory tests are performed and then the same experiments are numerically replicated in DEM. The article presents calibration of the DEM input parameters on the example of perlite D18-DN Based on the performed calibration, the model of perlite transport in a screw conveyor has been shown.

Keywords: *discrete element method, modelling, computer simulations, calibration, bulk materials, perlite.*

Analityczne metody obliczeniowe parametrów konstrukcyjnych maszyn i urządzeń transportowych są często niewystarczające, zawłaszcza w przypadku transportu nietypowych materiałów sypkich. Pomocnym narzędziem numerycznym wspierającym proces projektowania i optymalizacji urządzeń do transportu materiałów sypkich jest Metoda Elementów Dyskretnych (DEM). Uzyskanie wiarygodnych wyników symulacji wymaga kalibracji parametrów wejściowych modelowanego materiału wykorzystując wyniki badań laboratoryjnych właściwości fizykochemicznych rzeczywistych materiałów. W artykule przedstawiono metodologię kalibracji modelu DEM na przykładzie perlitu D18-DN. W oparciu o przeprowadzoną kalibrację zaprezentowano możliwości zastosowania metody DEM do symulowania transportu materiału przenośnikiem ślimakowym.

Słowa kluczowe: *metoda elementów dyskretnych, modelowanie, symulacje komputerowe, kalibracja, materiały sypkie, perlit.*

1. Introduction

Optimization of the design of machines and devices for the transport of bulk materials is aimed at reducing the costs of their production while maintaining quality and functionality. This process involves the analysis of the functional features of the device and the search for possibilities of its cheaper generation or improvement of functionality through structural improvements, saving or substituting of construction materials. There are some of the main optimization criteria adopted by design offices and companies producing industrial transport equipment like reducing the weight of the device, energy consumption and increasing productivity. The analytical approach to the design of machines and transport devices allows satisfactory accuracy to choose the characteristic dimensions of components, to predict efficiency and power demand, and to estimate the strength and durability of the device. However, this approach does not provide any information about behavior of the bulk material during transport and interactions with equipment. This knowledge is necessary to be able to start the process of design optimization. Computer-Aided-Engineering tools are helpful in this extent. Increasing computing power of computers allows the use of numerical methods to solve complex engineering problems. In the field of bulk material simulation, the Discrete Element Method DEM is widely used [2-3, 6, 9, 12]. It allows to simulate the behavior of granular materials with any physical properties subjected to various extortions results from the operating conditions of the considered device. An example of a DEM application in the conveyor belt simulation is shown in Figure 1.

Considering the simulation model the physicochemical and mechanical properties of the transported granular material requires calibrating the input parameters of the model (among others determining: coefficient of friction, bulk density, shape and size of particles) based on the results of laboratory tests [4-5,10-11,13]. This paper presents the methodology for testing bulk materials in terms of their use for the calibration of the model created in the DEM environment and the calibration process on the example of granular material – D18-DN perlite.

(*) Tekst artykułu w polskiej wersji językowej dostępny w elektronicznym wydaniu kwartalnika na stronie ***www.ein.org.pl***

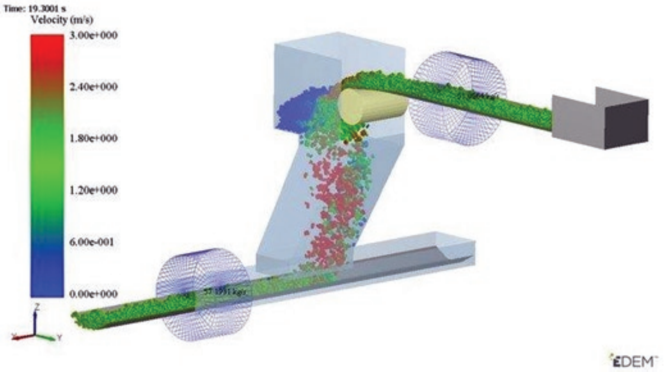

Fig. 1. An example of the application of the DEM method in belt conveyor simulations

2. Physicochemical properties of the material: D18-DN perlite

The simulation model of the material transport process requires properly defined parameters describing the physicochemical properties of the transported material. These parameters were determined on the basis of the laboratory tests results of D18-DN perlite. The scope of research included designation:

a) relative density of the material – ρ_{mat} [g/cm^3],
b) bulk weight – ρ_b [g/cm^3],
c) angle of natural repose – α_u [°],
d) outer friction coefficient of the steel-perlite friction pair – φ_z [–].

2.1. Determination of relative material density

The relative density of the material was determined by the pycnometric method. Measurements were made with a 50 cm^3 Gay-Lussac pycnometer. In the pycnometric method, distilled water is most often used as the standard liquid. Due to the chemical properties of perlite (the possibility of leaching in the aquatic environment), anhydrous ethyl alcohol was used as the standard liquid. The density value of the tested material was determined from the relation (1):

$$\rho_{mat} = \rho_{alk}^{t} \cdot \frac{m_3 - m_1}{(m_2 - m_1) - (m_4 - m_3)} \tag{1}$$

where:

ρ_{mat} – material density [g/cm^3],
ρ^{t}_{alk} – density of ethyl alcohol at temperature t [g/cm^3],
m_1 – weight of an empty pycnometer [g],
m_2 – weight of a pycnometer with alcohol [g],
m_3 – weight of the pycnometer with the material [g],
m_4 – weight of a pycnometer with alcohol and material [g].

The calculations include the change in the relative density of ethyl alcohol as a function of temperature. The mean value obtained from three measurements was taken as the relative density value of the examined materials.

2.2. Determination of material bulk density

The bulk density is the ratio of the weight of the material to its total volume, taking into account pores, spaces between the grains and any contaminants. The bulk weight of the material in the loose state depends on the specific weight of the material, its moisture content and the degree of filling of the given volume. The measurement was carried out in a measuring container with a volume of 1 dm^3, determining the bulk density of the material in the loose state ρ_b from the relation (2):

$$\rho_b = \frac{m_{2b} - m_1}{V} \quad \text{[g/cm3]} \tag{2}$$

where:

ρ_b – bulk density in the loose condition [g/cm^3],
m_{2b} – weight of the measuring cylinder and samples in loose condition [g],
m_1 – weight of the measuring cylinder [g],
V – capacity of the measuring cylinder [cm^3].

The average value obtained from three measurements was taken as the bulk density value of the tested materials.

2.3. The angle of natural repose

The angle of repose α_u is the inclination angle between descent of the material cone formed by free pouring and horizontal plane. The tests were carried out in a measuring stand with a loose charge of the tested material. The value of the angle of repose was directly measured at the test stand, and the photos which were taken for further analysis. Using the image analysis, the angles of material placement with respect to the horizontal plane were determined (Fig. 2.).

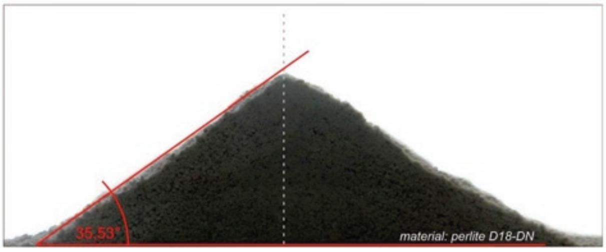

Fig. 2. Measurement of the angle of natural repose of perlite by using image analysis

2.4. Outer friction coefficient

Determination of outer friction was carried out in the AB-2A direct shearing apparatus used for soil cohesion studies. The tests were carried out in a 60 x 60 mm box at a normal stress of 500 kPa. Sample of material was subjected to normal stress and displaced into horizontal direction due to the horizontal force. On the basis of registered time characteristics or changes of the shear force value in the displacement function, the outer friction coefficient was determined from the relation (3):

$$\phi_z = \frac{F_S}{F_N} \tag{3}$$

where:

ϕ_Z – outer friction coefficient [–],
F_S – shear force [kN],
F_N – normal force [kN].

An example of registered changes of the shear force value in the displacement function is presented in figure 3. The calculations were carried out assuming the maximum tangential stress value or the tangential stress value corresponding to the box displacement by 6 mm (10% of the box dimension).

The results of the physicochemical properties of the model material – D18-DN perlite – are presented in Table 1.

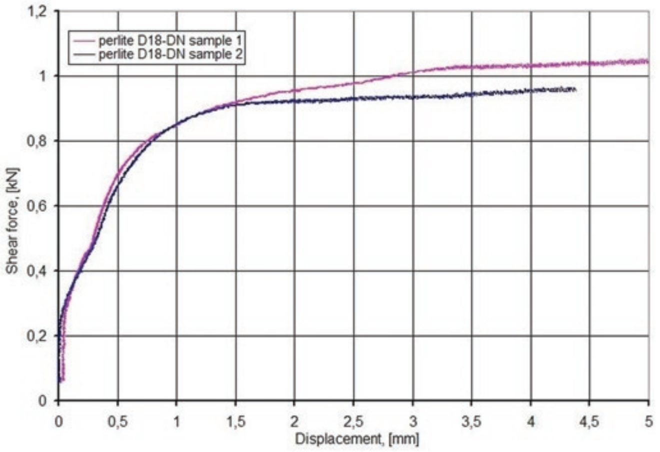

Fig. 3. Change of shear force as a function of displacement for a steel-perlite friction pair

Table 1. Physicochemical properties of D18-DN perlite

Physicochemical property	Value
Relative density ρ_{mat} [g/cm^3]	1.24
Bulk density ρ_b [g/cm^3]	0.10
The angle of natural repose [°]	35.50
Outer friction coefficient (friction pair steel-perlite D18-DN)	0.54

3. Description of the DEM method

Computer-Aided-Engineering programs have become important tools used by engineers in the process of designing new machines and devices in recent years. A number of engineering and scientific issues, which are too complicated to be described by analytical models or difficult to test in the laboratory, have been solved using numerical methods [1,7-8,14-15,17-18]. In addition, relatively cheap and easy access to high computing power and rapid development of computer programs implementing specific numerical methods causes that physical phenomena are modeled with incredible accuracy in relation to reality. The fundamental example is the Finite Element Method, which is commonly used to solve the problems of continuum mechanics (continuum). The base of the FEM method is the assumption that the modeled material is considered as a continuous in the macroscopic sense, and therefore it is characterized by a continuous distribution of matter (mass) in space, while its properties resulting from the atomic (or microscopic) structure are neglected. The idea of Finite Element Method is to divide the considered continuous area into a finite number of sub-areas (elements) connected to each other at nodes. In addition, it is assumed that the continuity of the center is preserved under load, hence the concept of FEM excludes its use in simulating the behavior of bulk materials. Therefore, for the needs of mechanics of discontinuity, the Discrete Element Method was developed. In DEM the considered material is modeled as a set of individual particles interacting with one another through appropriate contact models. Hence, the macroscopic features of the material are determined by the accepted properties of the particles and their interactions [19].

The algorithm of the DEM method is based on the contact mechanic, where forces acting on particular particles are calculated by appropriate models. Based on Newton's motion equations, particle accelerations are calculated. The velocities and positions of particles are determined by integration over time of these equations. By definition, the particles are rigid solids. However, the DEM method takes into account the deformation of particles in an artificial way, namely during the collision the depth of mutual penetration is calculated, as shown in Figure 4.

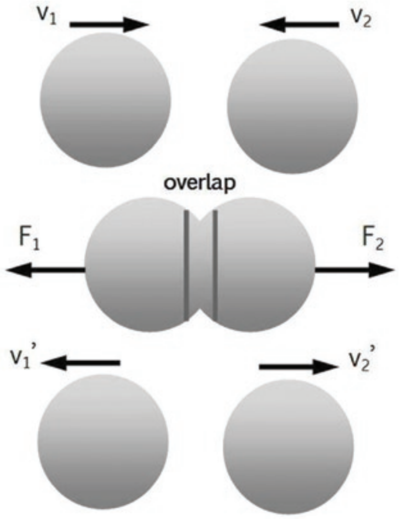

Fig. 4. Collision of rigid particles

The purpose of the contact model is to link the depth of penetration (in the normal and tangential direction in regard to the colliding particles) with the magnitude of contact force. Figure 5 shows the contact model of two particles during the collision. Usually, DEM simulation software offers a range of different contact models that allow modeling of elastic and plastic collisions with or without cohesion.

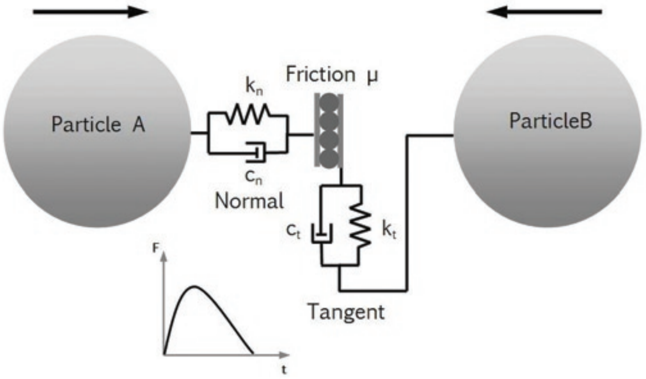

Fig. 5. Contact model of two particles during a collision

The parameters of individual particles (size, shape, density) and contact parameters (coefficients of friction, rolling resistance, coefficient of restitution) have a large influence on the behavior of the modeled bulk material [4]. The basic shape of the DEM particle is the sphere, however, due to the fact that the actual shapes of individual grains rarely take the ideal, spherical form, it is possible to create more complex shapes as a result of permanent connection of spherical particles. However, it has to be noted that the use of very complex shapes of clumps results in the extension of the calculation time.

Therefore, it is important to find a compromise between the actual shape and size of the solids, and those used in DEM simulations. To provide reliable behavior of the material in DEM simulations, the input parameters of the model should be calibrated (i.e. friction coefficients, density, etc.).

4. Calibration of DEM parameters

In DEM analyzes, both physical and contact parameters are defined at the microscopic level of the particle [16]. Calibration consists in selecting of input parameters on a micro scale to obtain a convergent result of the modeled soil with the behavior of the real soil (macro scale). Therefore, it is more important to accurately reproduce the behavior of the entire soil than individual particle interactions. Parameters are calibrated by performing a suitable laboratory tests, e.g. measuring of the angle of repose or shear test. Then the same experiment is modeled in the DEM environment. Assuming a specific shape and size of particles, an iterative selection of the input parameters of the model is made until the convergent result with the experiment has been obtained [19]. As part of this work, the process of calibration of DEM input parameters has been presented on the example of laboratory measurements of physicochemical properties of perlite D18-DN.

Calibration of the DEM model begins with the selection of the shape and size of the particles. There is no unambiguous rule how to simplify the modeled shape of a solid and how to accept its size. A number of simulation studies performed by many researchers indicate that this selection is dictated by the specific purpose of the simulation. Both complex clumps and spherical particles are able to reflect the real angle of repose. In the case of spherical particles, an additional coefficient limiting the rolling of spheres should be introduced in the DEM model. An important factor in DEM simulation is the calculation time, which is influenced, inter alia, by the number of particles used and their size (in accordance with Rayleigh's theory). In the case of fine materials or powders, the dimensions of DEM particles are scaled so as to provide a reasonable compromise between the accuracy of the calculation and the runtime of simulation. Typically, the particle size of the modeled material is selected based on the proportions of the characteristic dimension of the device (e.g. screw pitch) to the particle radius.

Taking into account the regular shape of the perlite, spherical particles with 2, 5 and 8 mm radii were assumed. Sizes have been scaled relative to the actual grain dimensions to reduce their number in the soil, thereby limiting the calculation time. Due to the fact that perlite does not show cohesive properties, the simulation uses a non-linear contact model according to the Hertz-Mindlin theory. Then, bulk density calibration was performed for each particle size. It consisted of free filling up a measuring cylinder of a specified volume and evaluating the mass of the material in the filled cylinder space (Fig. 6). The input parameter of the model was the actual density of a single particle. This density was selected in an iterative manner to receive a value of bulk density convergent with obtained one as a result of laboratory measurements. The results of the above analysis also provided information on how the size of the selected particle influences the value of the bulk density. Table 2 presents the results of the bulk density depending on the particle's radius and the actual density.

The study of the angle of natural repose was aimed at calibrating the contact parameters of the model, i.e. the coefficient of internal friction and rolling resistance. In the DEM simulation, the laboratory test stand for examining the angle of repose was replicated [10]. The calibration consisted of an iterative selection of the values of both coefficients (inner and rolling friction), which made it possible to obtain the natural angle of the perlite close to the real one. For this purpose, a research plan was adopted consisting in changing the value of only one input parameter, i.e. the coefficient of internal friction at

Table 2. Calibration results of perlite bulk density

Particle radius [mm]	True particle density [kg/m^3]	Bulk density [kg/m^3]
2	200	119.4
5	200	119.9
8	200	119.7

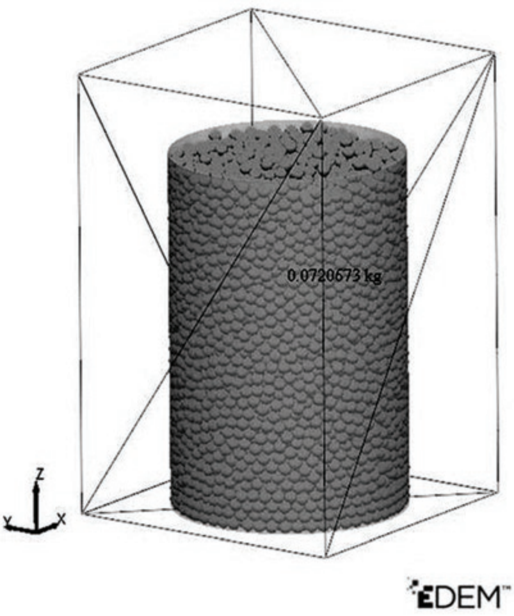

Fig. 6. Calibration of bulk density

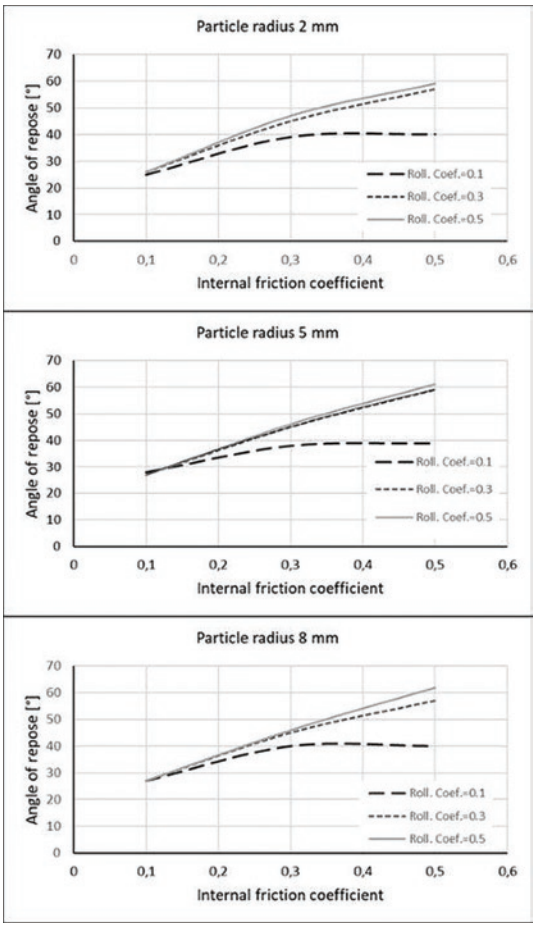

Fig. 7. The influence of the input parameters to the value of the angle of natural repose

a constant value of the rolling resistance coefficient. The series of simulation tests was repeated for three values of the rolling resistance coefficient. In results, characteristics combining the coefficients of internal friction and rolling resistance with the value of the angle of repose were obtained. Figure 7 presents graphs of changes in the angle of repose depending on the assumed input parameters.

Figure 8 shows the calibrated repose cone. This approach, assuming three different particle radii, three levels of internal friction coefficient and three values of rolling resistance coefficient, requires 27 simulations. These studies are undoubtedly time-consuming, but they provide important information about which input parameters determine the value of the angle of repose. Calibration of the outer friction coefficient (material-steel) was made on the model of a box apparatus for direct shear testing of the soil.

The model of the DEM test stand is shown in Figure 9. A sample of calibrated material was placed inside the box bounded from the bottom by a stationary plate and from the top by a stiff punch generating pressure on the material. Through the iterative change of the friction coefficient of the material-plate contact pair and the registration of the change of the normal and tangent force, it was possible to estimate (due to the relation 3) the outer friction coefficient.

The influence of the coefficient of friction in the micro scale on the value of the coefficient of friction in the macro scale is presented in Figure 10.

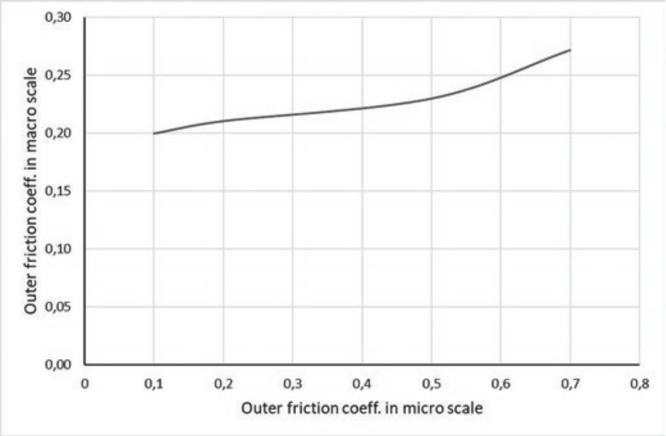

Fig. 8. Calibrated angle of natural repose

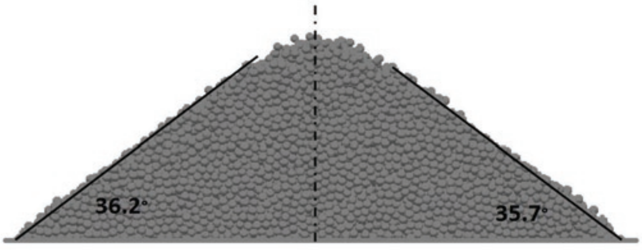

Fig. 9. Calibration of the outer friction coefficient

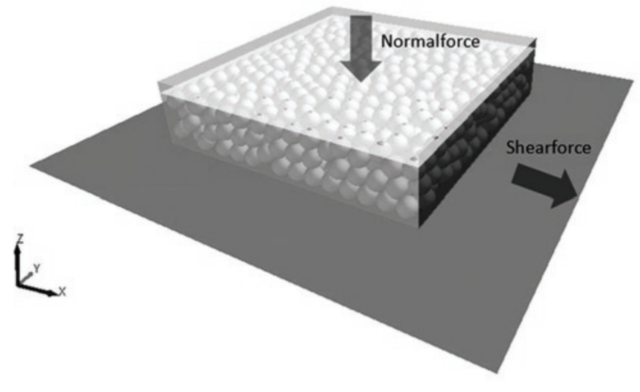

Fig. 10. Dependence of the outer friction coefficient on the deposit on the friction coefficient of a single particle

5. Simulation of transport of D18-DN perlite in a screw conveyor

By having properly calibrated input parameters of the DEM model, it can be started performing the right simulations. Simulations can be used, among others, to determine the expected transport performance of the designed device or to determine the required drive power. The following is an example of a simulation of the transport of D18-DN perlite in screw conveyors. Two screws with the same external and internal diameters, differing only in the dimension of the pitch, were analyzed. Variant 1 that was assumed is a screw with a pitch of 250 mm and variant 2 - a screw with a pitch of 150 mm. The basic geometrical dimensions are shown in Table 3.

The results of the simulation provided information how the screw pitch influences the efficiency and power demand at different rotational speeds of the shaft. For the analysis, 5 mm particles were selected. The simulations for both variants of the screw were made by changing its rotational speed in the range of 10-70 rpm. The model of the screw conveyor with the material is shown in Figure 11.

Table 3. Parameters of the analyzed screw conveyors

Screw variant	External diameter [mm]	Internal diameter [mm]	Screw pitch [mm]
Variant I	250	139	250
Variant II	250	139	150

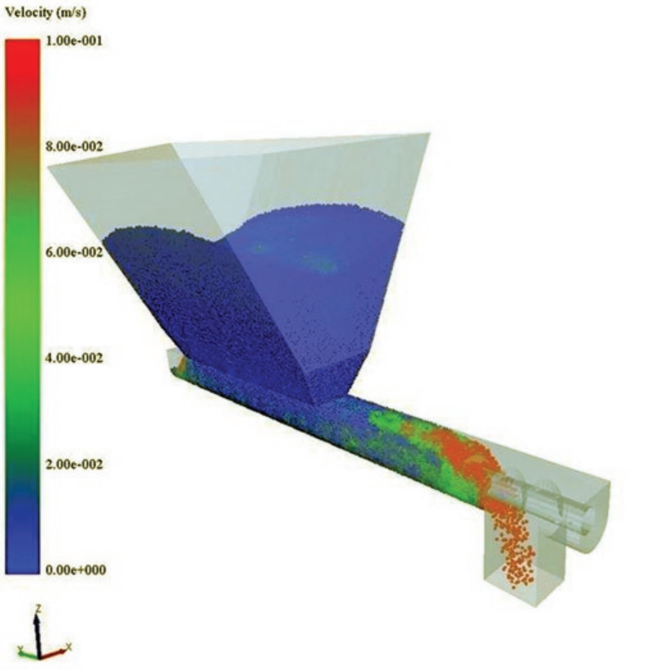

Fig. 11. Model of the screw conveyor

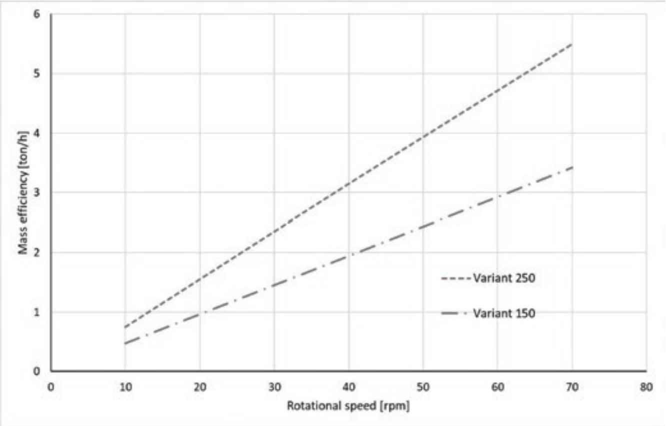

Fig. 12. Mass efficiency of the conveyor depending on rotational speed and screw pitch

The simulation results for both conveyor variants showing the mass efficiency depending on the rotational speed of the screw pitch are shown in Figure 12.

The change in the helix of the conveyor directly affects its transport efficiency. With increasing pitch at the same rotational speed of the shaft, mass efficiency increases. Having an adequately correlated material model, one can easily examine the functionality of a given transport device or select its appropriate geometric dimensions. In addition to determining geometrical characteristics, it also can be determined the required drive power. Figure 13 presents the demand for the power of the screw conveyor depending on the rotational speed and pitch of the screw in both accepted variants.

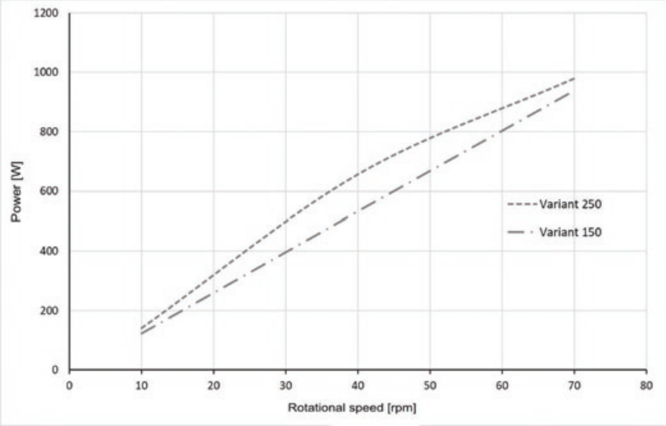

Fig. 13. Demand for the power of the conveyor depending on the rotational speed and screw pitch

From the graph above, it can be seen that the need of the conveyor for power increases with the increase of the rotational speed. For the same rotational speed of the shaft, reducing the screw pitch results in a reduction of the power demand. The increase in power demand is not directly proportional to the increase of mass efficiency, which is particularly visible at shaft speeds above 50 rpm. For example, at a speed of 70 rpm and a change in pitch from 150 mm to 250 mm, mass efficiency increased by 60%, while the power demand increased by only 6.5%. With the characteristics of the device's operation, it is possible to optimize the dimensions and mass of the screw or determine the preferred speed range. This speeds up the design process and allows for virtual testing of various solutions.

6. Conclusion

The process of calibration of input parameters of the DEM model is a factor that strongly determines the reliability of the final results of the simulation of the flow of bulk materials in transport machines. Laboratory tests determining physical and chemical properties of materials are relatively easy and cheap, especially in the case of fine-grained materials. This is undoubtedly a huge advantage, because on their basis numerical model can be calibrated. As demonstrated by the DEM calibration process itself, due to the iterative selection of individual parameters, it is a time-consuming process. Simulation tests have proved that the radius of a spherical particle does not affect the bulk density of the soil. Therefore, one size of spherical particles can be using. Likewise, the size of the particles does not substantially affect the value of the angle of repose. The above tests show that the same value of the cone angle can be obtained by using different sets of parameters of the internal friction coefficient and the coefficient of rolling resistance. The values of rolling resistance coefficients such as $F = 0.3$ and $F = 0.5$ have a slight influence on the value of the angle of repose. Different results were obtained by assuming the rolling resistance coefficient $F = 0.1$. In this case, for all three particle diameters (2, 5 and 8 mm) assumed in the simulations with an increase in the internal friction coefficient μ_w value of the angle of natural repose α_u initially grows and then assumes a constant value $\alpha_u \approx 40°$ for $\mu_w \geq 0.3$. This phenomenon can be explained by too low moment of rolling resistance of particles causing their rolling along the slope of the cone. This means that even with a very high value of the internal friction coefficient, the angle of repose will be small. Hence, in the case of spherical particles, it is necessary to use a rolling resistance model with an appropriate value (calibrated). The outer friction coefficient of soil depends non-linearly on the value of the single particle coefficient.

The DEM material model calibrated in this way should be verified by simulating a specific application, e.g. transport in a screw conveyor. As comparative features, the device operating parameters should be determined, i.e. screw shaft torque, mass efficiency or power consumption, which can be confronted with the results obtained on the laboratory line. In addition, further simulation studies should focus on non-spherical particles due to the fact that real solids have more complex shapes.

Undoubtedly, an important advantage of DEM simulation is the ability to quickly compare several constructions in terms of accepted criteria, e.g. transport efficiency or power. Quantitative and qualitative assessment of these differences allows for a proper selection of geometric features of the screw conveyor transporting a specific type of bulk material. This improves the design process and allows to explore different configurations without having to make expensive prototypes of devices.

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