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DEM investigation of the effect of arrangement of grains on the behavior of brittle granular materials subjected to one dimensional compression

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ABSTRACT: Granular materials are used in many projects such as dams, railways and breakwaters. Because the size of granular materials in these projects starts from a few centimeters and sometimes reaches one meter, conducting laboratory experiments would be very expensive, time-consuming and even impossible. For this purpose, the use of numerical modeling to investigate the effect of different parameters on the mechanical behavior of this type of material is very important. Among the effective factors, grain arrangement is investigated in this study. Thus, cylindrical and cubic grains are modeled as representative of rounded and angular grains, in two regular and irregular arrangement based on the discrete element method and stress-strain behavior, applied energy and breakage values after loading are investigated. Using the non-linear Hertz model and determining its parameters based on laboratory experiments, controlling the uniformity of grain distribution based on the number of contact points along with the dip and direction of grains, defining the breakage criterion based on Von-Mises criterion and applying the breakage pattern based on particle splitting are among the features of the model used. In order to validate the numerical model, similar laboratory experiments were performed and their results were compared with each other. The results showed that the numerical model can study the effect of the arrangement of grains on the behavior of materials with high accuracy. Also, due to the existence of different shapes in granular materials, the effect of mixed arrangement was investigated on the results.

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1- Introduction

The performance and stability of structures such as earthfill and rockfill dams, railway ballasts and breakwaters are related to the shear behavior as well as the breakage of the aggregates. In general, many parameters affect the behavior of granular materials, including: stress state, grain size and shape, grain size distribution, grain density, fracture toughness, friction between grains and water content [1]. In real conditions, the size of granular materials used in structures such as dams varies from a few millimeters to several tens of centimeters [2]. In the ballast of the railway, the size of the grains is generally between 1 to 7 cm [3]. This makes laboratory tests on such materials very expensive and time-consuming and even impossible in some cases. On the other hand, it is practically impossible to apply the same initial conditions to the experiments in terms of size, shape and position of the grains relative to each other. All of these limitations lead to the use of numerical modeling in the analysis of the behavior of brittle aggregates.Various researches on the behavior of granular materials have been done through numerical modeling [4-6]. Based on previous studies, using the discrete element method, the mechanical behavior of granular materials in different conditions of size, shape and loading conditions can be obtained and analyzed. But the important issue is the adaptation of the modeled grain to its actual shape. On the other hand, in the latest studies conducted in the years 2020 to 2022, the grains have always been randomly placed inside the loading chamber and the only controlling parameter has been the porosity of the grains. For spherical grains, porosity control is sufficient, but if the modeled grain is non-spherical, then the slope and direction of the grains and the type of contact between the grains will greatly affect the behavior of the material. In this regard, Zhang et al. In 2020 [7] modeled the combined arrangement of grains with different shapes. They modeled only one combined arrangement and compared the results with the uniform arrangement of spherical grains. In his work, the effect of changing the grain combination with different spherical coefficients on the stress-strain behavior of the grain set has not been investigated.In this study, to investigate the effect of shape, the grains are modeled in two cubic and cylindrical shapes, in two different sizes that are exactly similar to laboratory experiments. To investigate the effect of slope and direction of grain placement, two conditions of regular and random arrangements of grains are also modeled and then the results are compared with the

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Table 1. Geometrical properties of the grains and loading conditions

	Cube A	Cylinder A	Cube B	Cylinder B
Dim.	12×12×19	14×20	27×27×27	25×27
S	0.31	0.54	0.57	0.69
Load (kN)	50, 100, 150		150, 213, 300	

relevant laboratory results. Finally, after numerical modeling validation, two combinations of cubic and cylindrical grains with different percentages of shapes are modeled and their stress-strain behavior at high-stress levels is evaluated.

2- Methodology

In this study, to investigate the effect of shape, two groups of cylindrical and cubic grains, each in two different sizes were selected as representative of angular and rounded grains, respectively (Table 1). The sphericity coefficient (S) of these grains is determined as the ratio of the radius of the largest circumferential circle (r) to the radius of the smallest circumferential circle (R).

Hertz nonlinear model was used to determine the contact behavior between the grains. Then, the number of balls required to form each clump was obtained using sensitivity analysis. The grains were then placed inside the loading cell in two regular and irregular arrangements. In the irregular arrangement, the number of contact points of each grain with adjacent grains along with the slope and orientation of the grains were controlled to ensure that the initial conditions of the experiments were the same. Then the tensile strengths of cubic and cylindrical grains were assigned based on their corresponding strength distribution diagram. To evaluate the possibility of grain breakage, the von-Mises criterion was used. It should be noted that the grain strength values are modified based on the confinement caused by adjacent particles at each time step. If the breakage criterion is met, each grain must break according to a predetermined pattern. In this study, it is assumed that each grain is divided into two parts due to breakage; In such a way that the resulting shape is as similar as possible to the original shape of the grain.

3- Results and discussion

In this paper, stress-strain curves, input energy per unit volume of the grains and breakage factor were determined. It should be noted that the strain in this paper is the relative displacement of the loading plate relative to the initial height of the loading cylinder. It was observed that the diagrams obtained from numerical modeling were more than 90% consistent with the relevant laboratory results. Nonlinear hardening behavior was also observed in all experiments. In general, the stress-strain behavior of materials can be divided into two parts. In the first part, which deals with the initial rearrangement of the grains, for small amounts of applied stress, the grains slip and move and reach to the threshold state. The amount of strain in this condition varies for different grains. In the second part of the diagram, the values of stress increments increase with respect to strain increment and hardening behavior occurs. Comparing the behavior between specimens of the same size but in different shapes in irregular arrangement, it was observed that the amount of strain occurred for the cylindrical grains of type A was about 17% higher than the cubic grains of type A. However, in group B grains, whose average volume is more than 5 times the average volume of group A grains, the displacement values of cubic specimens were about 11% higher than the corresponding values in cylindrical specimens.In regular arrangement, only breakage can occur in the grains. Because there is an area contact between the cubic grains and a linear contact between the cylindrical grains, and this prevents corner breakage and lip filling in the grains.An important parameter that should be considered in reviewing the results and validation of the numerical model in the uniaxial load test is the breakage factor. Breakage factor values obtained from numerical modeling, with an error of less than 20%, were able to predict the actual values of breakage that occurred in laboratory experiments. In the case of irregular arrangement, cubic specimens of both sizes experienced, on average, 18% more breakages than cylindrical grains. The reason for this depends on the lower sphericity of the cubic grains and the greater stress concentration in them.The results of grain combination modelings showed that by increasing the amount of cubic grains and decreasing the total sphericity coefficient, a higher percentage of grains broke.

4- Conclusions

In a fixed arrangement and the same state of contact between the grains, the angular the grains and the more the material moves away from the spherical shape, the higher the breakages due to the concentration of stress. Cubic grains experienced an average of 18% more failure than cylindrical grains.

In regular arrangement, the position of the grains next to each other (whether the grains have a linear or area contact) affects the breakage factor more than the grain shape.

In regular arrangement, there is no possibility of slipping and rotation of the grains and the mechanical performance of the grains is only breakage. In irregular arrangement, however, in addition to the possibility of breakage, the grains can be displaced. Thus in regular arrangement, grain breakage begins at lower stress values than in irregular arrangement.

In the case of irregular arrangement, the amount of breakage factor for all shapes increases with increasing grain size. This is due to the presence of more microcracks in larger grains, which reduces the strength and increases the breakage in them.

In this study, only the effects of breakage in the form of splitting have been applied. It is possible to increase the accuracy of modeling by completing future research in the form of modeling corner breakages and edge fillings that occur at low stresses.

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