UNIAXIAL COMPRESSION A SOFT GRAIN COMPOSED OF AGGREGATE PRIMARY PARTICLES

MÔ HÌNH SỐ QUÁ TRÌNH NÉN MỘT TRỤC CỦA HẠT MỀM ĐƯỢC CẤU THÀNH TỪ TẬP HỢP CÁC HẠT SƠ CẤP

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Abstract - Deformable materials such as latex rubber, clays, and concrete are commonly used in civil construction, that can large deformation. This paper uses the discrete element method to simulate a soft grain that can deformed without rupturing. This soft grain is composed of rigid primary particles with a cohesive contact law between them. The results showed that rigid primary particles within the deformable grain can move and rearrange in response to vertical compression. The soft grain is characterized by a linear response to small deformations and plastic behavior beyond, on the other hand, the axial stress as a function of the cumulative axial deformation for a grain undergoing vertical compression followed by a discharge from 10% and 30% deformation.

Key words - Discrete element method; soft grain; large deformation; cohesive force.

Tóm tắt - Vật liệu biến dạng hiện nay được áp dụng và sử dụng phổ biến trong lĩnh vực xây dựng như là: cao su, đất sét hay là bê tông, trong đó các vật liệu này có khả năng biến dạng lớn. Trong bài báo này, sử dụng phương pháp phần tử rời rạc để mô phỏng quá trình biến dạng mà không bị phá hủy của mẫu vật liệu bằng phương pháp nén một trục theo chiều đứng. Mẫu vật liệu này được xây dựng trên tập hợp các phần tử nhỏ, được liên kết với nhau bằng lực dính kết. Kết quả cho thấy, các phần tử nhỏ di chuyển và sắp xếp các vị trí của nó trong mẫu vật liệu khi chịu nén. Biến dạng của mẫu hạt mềm là đàn hồi trong giai đoạn đầu khi biến dạng nhỏ, tiếp sau đó là biến dạng dẽo, mặt khác, ứng suất dọc trục là một hàm của biến dạng dọc trục tích lũy khi thực hiện tháo tải ra tại thời điểm mẫu bị biến dạng 10% và 30%.

Từ khóa - Phương pháp phần tử rời rạc; hạt biến dạng; biến dạng lớn; lực dính kết

1. Introduction

The mechanical behavior and the textural properties partly reflect the weakly deformable character of the particles in the granular media studied. For example, the heterogeneous distributions of forces are linked to small areas of contact between particles (which makes it possible to assimilate them to point contacts) and to steric exclusions. Likewise, plastic behavior and memory loss from the initial state to the critical state result from rearrangements of particles and energy dissipation through friction and inelastic collisions. However, there is a large class of materials with the particularity of being composed of soft grain, defined as particles which can undergo large deformations without fracturing [1-3]. Given the known properties of hard particle granular media, the central problem in the study of these materials, which we will call Soft Particle Materials, is to understand to what extent their properties depend on the deformability of the particles especially within the limit of large particle deformation and high compactness [2], [4-7].

The constituent particles of all these materials are macro-molecular or granular aggregates, with sizes between 1 nm and 1 mm. They may be divided into four groups according to their composition and structure: surfactant particles, polymer-colloid systems, lattice particles, and colloidal-type particles [3]. On the other hand, granular materials composed of loose aggregates, and metallic wear particles are produced by the friction between solid bodies (called "third body" in tribology) during the hot forming process [8]. Compaction of soft powders has become a well-established manufacturing process for metals and monolithic polymers, allowing components to be produced with appropriate dimensional tolerances [9].

The large deformations of a single soft particle and the interactions between two particles depend on the nature of the material and the shape of the particle. The particles studied are essentially spherical in shape. There are now several models for large deformations of simple solid particles such as homogeneous solid spheres, spherical membranes filled with an incompressible fluid, and elastic spherical shells as well as the Tatara's model for rubber spheres predicts [10], [11], Lin et al., investigated the deformation of soft spherical particles under vertical compression [12], and soft glasses of Bonnecaze et al. [3] However, shells and spherical membranes are more complex insofar as the deformation depends on the compressive and bending moduli and therefore on the thickness of the wall [13]. When it comes to elastoplastic spheres, the plastic deformation starts at the contact zone's boundaries and continues as long as the stress in these areas stays at the plastic threshold. In the Bonnecaze's model, Soft Glasses are the assemblage of soft particles in a periodic box. The results obtained are in good agreement with the experiment. However, the soft particles can overlap largely between particles when they contact in that model.

In this paper, we defined a Soft Particle as composed of an assemblage of the primary particles, which can undergo large deformations without breaking and interacting thanks to low potentials which can be regulated through their chemical composition. When interactions between the primary particles occur, they are governed by a cohesive contact law. We use the discrete element method to simulate this soft particle. We will discuss the characteristics of particles in this material below.

2. Numerical approach

In this paper, we use the Bonded Particle Model (BPM) to model the deformable grain in which each deformable grain is represented by the rigid primary particles with cohesive interactions [14], [15]. The external forces operating on the boundaries of the deformable grain can cause the primary particles to move and rearrange. In this model, we use the cohesive attractions between the rigid primary particles to prevent the dispersion of the primary particles while allowing their displacements and rearrangements. Under effect of the external forces, the grain undergoes a rupture and can break into pieces. To allow larger deformation and to avoid fragmentation, the choice a contact interaction law is necessary. Here, we consider that this law includes a short-distance repulsive force with a long-range center-to-center attraction force as in colloidal systems [16], [17]. So, the interaction force F is composed of two forces: the first is the attractive force F_a and the second is the repulsive force F_r.

For the attractive part of the interaction between the primary, we call the radii r_1 and r_2 of two rigid circular particles separated with a distance δ. Hence, this interaction force is defined as a power law with an exponent γ in the attraction part of the Lennard-Jones' force.

$$F_a = -F_0\left(1+\frac{\delta}{a_0}\right)^{-\gamma} \quad (1)$$

Where $a_0 = r_1 + r_2$, and δ is the distance between particles. So, the maximum of this force will be F_0 when the distance between particles is null ($\delta = 0$).

Only when two particles come into contact, specifically when $\delta = 0$, as shown by the red line in Figure 1, does the repulsive force F_r become active. Thus, at the end of attraction at an arbitrary distance $\delta > 0$, the interaction force $F = F_a + F_r$ as a function of δ is lowered and takes on a value $\in [-F_0, +\infty]$ upon contact ($\delta = 0$) [18], [19]. Figure 1 shows the graph of this interaction law for $\gamma = 2$ and $\gamma = 7$.

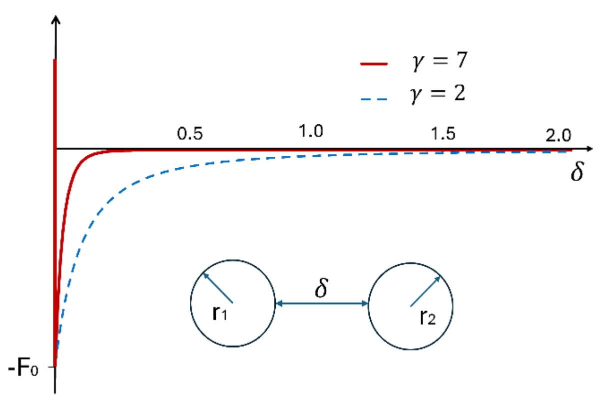

Figure 1. *The graph of the interaction law between two primary particles with two cases $\gamma = 2$ and $\gamma = 7$*

A cut-off at a specific distance is required for this law to be implemented effectively. Only the first and second neighbors of each particle interact with each other when $\gamma = 7$, as the force of attraction is insignificant beyond $\delta \simeq a_0$. Although it is brief, this distance is adequate to keep a particle's primary particles together throughout the quasi-static deformations. The BPM technique is described in detail in Nemabazadi's work [20]. The coefficient of friction between the primary particles is adjusted to zero in order to prevent the localization effects of deformation and volume fluctuations. In fact, each particle's volume is nearly constant when there is no friction coefficient between the primary particles since the rearrangements do not result in dilatancy [21]. As a result, the internal compactness of the particles remains close to that of a random assembly. Additionally, there is no longer material involved in the primary particle rotation within the grain, thus friction does not cause any internal energy dissipation. We have set the normal and tangential restoring coefficients to zero to allow energy dissipation during the rearrangements of the primary particles. This dissipation indirectly confers a rubbing character on the particles because the dissipation under the effect of shocks is proportional to the relative speed is therefore to the stress which is exerted on the particle.

Furthermore, due to mutual steric exclusions of the primary particles, a grain may be in static equilibrium with varying configurations of the primary particles. In other words, a BPM grain can take various forms and keep it when external forces are suppressed. Each grain's deformation not only contains a plastic component resulting from primary particle rearrangements but also a little reversible component caused by the action of the forces of attraction.

It should be noted that since the primary particles interact without friction, there is no need to add a friction force between the primary particles belonging to two separate particles. The friction force is never mobilized at such friction contacts because the rotations of the primary particles at the contact points are not coupled to the overall rotation of each particle. Such an effect can only be mechanically material if a rolling resistance between primary particles is added.

3. Results

Here, we investigate the precision and effectiveness of the suggested models by applying the previously mentioned method to the behavior of a grain.

As seen in Figure 2, we have carried out BPM simulation of a grain between two stiff walls with a radius of R = 5 mm. The top wall descends at a steady 0.2 m/s while the bottom wall remains still. The rigid primary particles that make up the grain in BPM simulations have diameters that vary arbitrarily from d_{min} to d_{max}. Equation (1) governs the interaction between the primary particles, with the values of the maximum tensile force of a pair of contacting primary particles (F_0), the diameter of the primary particles, an exponent γ. Table 1 contains a list of all the key parameters for our simulation.

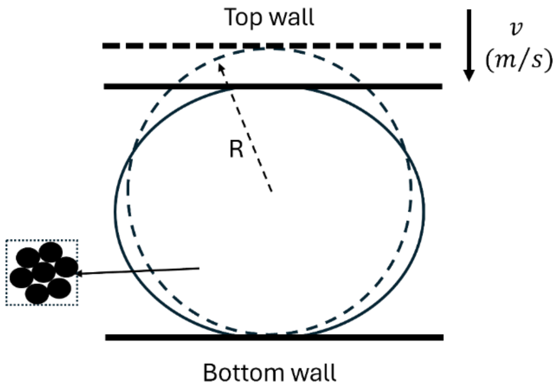

Figure 2. *A schematic drawing of the compression of a grain composed of the primary particles, in-dash line for an initial stage and in solid line for a deformation stage*

For a choice of the exponent γ, the law of interaction between primary particles comprises the two parameters F_0 and a_0, or in general, the size distributions of the primary particles. The choice of F_0 is not critical since the deformation of the particles is determined by the relationship between the external forces and F_0. It is more convenient to introduce the characteristic constraint $p_I = F_0/\langle a_0 \rangle$. If the confining pressure p of an assembly of BPM grain is less than p_I, so the particles do not deform much, and the system can be considered to be governed by particle rearrangements. If, on the contrary, $p/p_I \gg 1$, then the particles are strongly deformed, and the deformations are governed by those of the particles. The mechanical behavior therefore depends on the p/p_I ratio. It is absent from the behavior of an assembly of non-deformable and non-breaking particles. In this sense, p_I corresponds to the plastic threshold of BPM grain.

Table 1. *Principal parameters for BPM simulation*

Parameter	Symbol	Value	Unit
Number of rigid primary particles	N_p	1750	-
Grain radius	R	5	mm
Largest particle diameter	d_{max}	0.26	mm
Smallest particle diameter	d_{min}	0.16	mm
Maximum force when has not contact	F_0	100	N
Exponent coefficient of contact law	γ	7	

A grain deformed for a vertical deformation ε = 10%, 30%, and 50% is presented in Figure 3 (b), (c), (d) with force chains between the primary particles. We can observe that the contact area with the stiff walls forms a perfect contact line of the BPM grain, reflecting a plastic behavior of this particle. Consequently, the constraint inside a grain is almost homogeneous in the BPM grain (except for local inhomogeneities of the chains of force).

Figure 4 shows the vertical stress $\sigma = F / L$ as a function of the cumulative axial deformation $\varepsilon = \ln(1 + d / R)$ where L is always the horizontal diameter of the grain.

The BPM grain demonstrates a linear response to small deformations of about 2% and plastic behavior beyond. The characteristic stress $p_I \simeq 0.5$MPa is nearly equivalent to the threshold plastic stress, which stays constant.

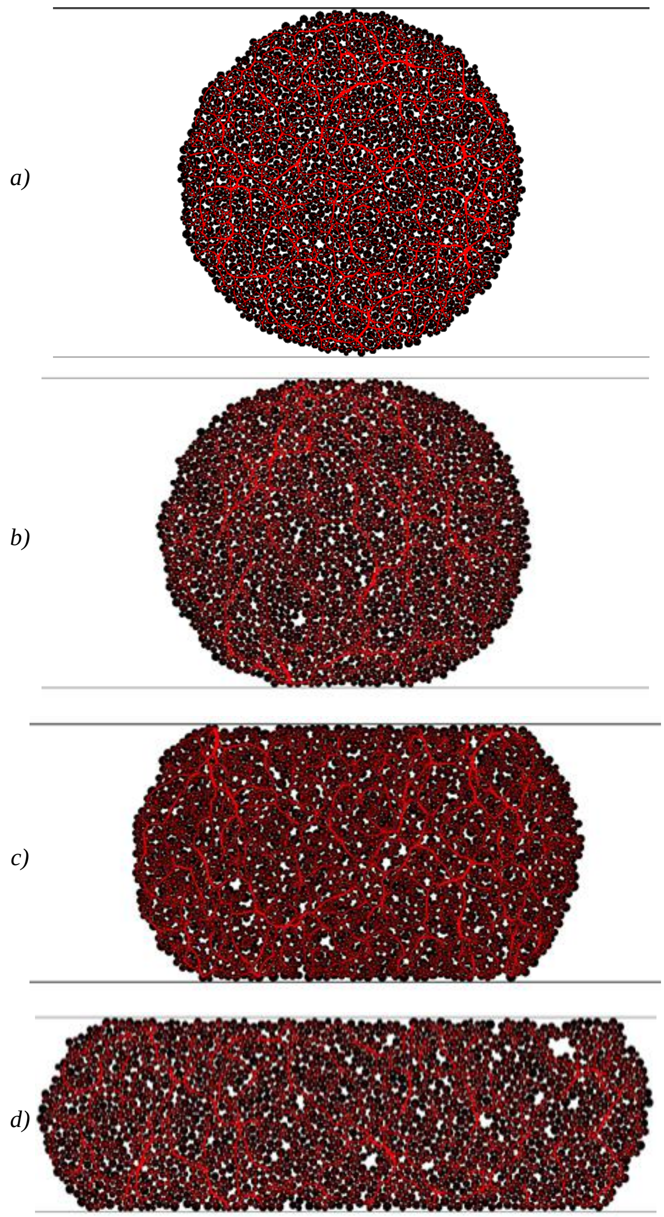

Figure 3. *Compression of a soft grain composed of the primary particles by BPM at the initial stage (a), at the vertical deformation ε = 10% (b), 30% (c) and 50% (d)*

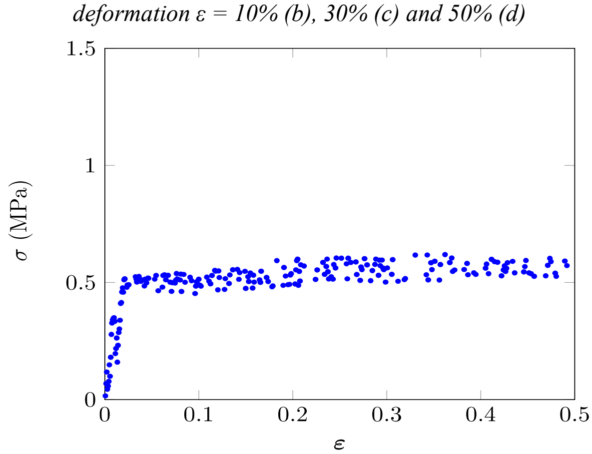

Figure 4. *Axial stress for a grain under compression as a function of total axial deformation*

The size distribution of primary particles only changes the internal compactness of a grain. The previous study showed the testing of the grains with different grain sizes, the deformations of the grains are a little smoother in the case of polydisperse size distributions [22], [23]. This is why, in most simulations, we have introduced a factor of two between the maximum and minimum sizes of the primary particles. Note also that the absolute value of a_0 is not crucial and only modifies the value of p_I. Finally, the accuracy of the model naturally increases with the number of primary particles per particle. Note that in 2D, several primary particles greater than 1000 make it possible, even in a very deformed state, to obtain a good representation of the shapes of the soft grains.

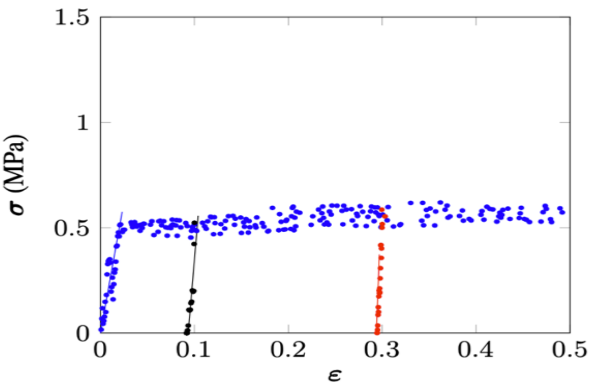

Figure 5. *Vertical stress is represented as a function of the cumulative axial deformation for a grain undergoing vertical compression followed by a discharge from 10% and 30% deformation*

To illustrate the plasticity of the BPM grain, we applied a discharge at two levels of deformation (10% and 30%). Figure 5 shows that stress decreases linearly during the discharge with a slope which seems to increase slightly with deformation. The grain deformed after a discharge from ε = 30% is presented in Figure 6 with chains of force. Note that, despite the chains of force present inside the particle, the average macroscopic stress after discharge is zero. The chains, in fact, only represent the repulsive forces on contact between primary particles. At equilibrium, these forces are compensated for by the mutual attraction forces between particles. The grain maintains its shape at equilibrium despite the cancellation of the applied constraints.

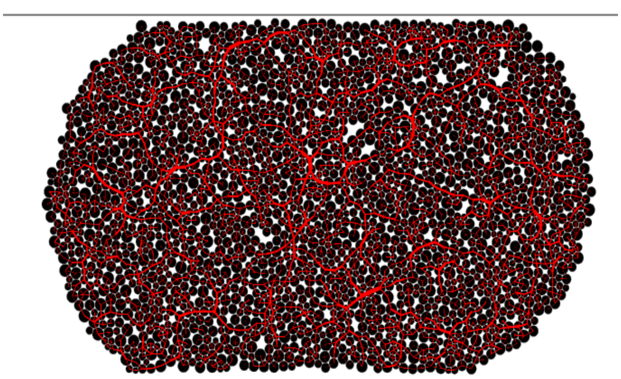

Figure 6. *An image of the BPM grain after the discharge from a vertical deformation of ε = 30%*

4. Conclusions

In this paper, we use the BPM model to investigate the behavior of soft-grain materials. Soft grain in this model is composed of rigid primary particles interacting through a force of attraction between the particle centers up to a cut-off distance on the order of a particle's diameter and a force of repulsion at the contact points. In this work, the repulsive force of contact is treated using the method of contact dynamics (CD). For the force of attraction, a Lennard-Jones force law is introduced.

The results showed that the BPM grains exhibit a linear response to small deformations and plastic behavior beyond a threshold that can be evaluated from interactions between primary particles based on the diametral compression of a grain. This may originate from the movement and rearrangement of the rigid primary particles in the deformable grain. Additionally, the axial stress as a function of the cumulative axial deformation for a grain undergoing vertical compression followed by a discharge from 10% and 30% deformation, is represented. These results show the BPM with soft grains significantly broadens the range of soft grain applications for DEM. By manipulating the interactions between primary particles, the behavior of soft grains can be calibrated or changed. Essentially, the fundamental particle interactions are just extremely strong repulsive potentials that exist between the molecules. Because of this, an attractive effective potential allows BPM to be applied to colloidal entities in interaction.

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