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Towards a mechanistic model for the interaction between plastically deforming particles under confined conditions: a numerical and analytical analysis

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Abstract

Triaxial compression of plastically deforming particles was studied with the finite element method in order to identify the mechanisms that underlie their mechanical response under confined conditions. In addition to the established elastoplastic behaviour at small and intermediate strains, the coalescence of plastic zones centred at contacts resulted in a reduced stiffness, whereas a significantly increased stiffness was seen once the material displaced by plastic deformation filled the ambient void space, signifying the onset of a stage dominated by elastic volume reduction. Moreover, an analytical model for multiple simultaneous contacts was formulated, assuming that the deformed particle shape could be approximated by a truncated sphere and that the behaviour of each individual contact could be described in terms of a hardness. The thus obtained model exhibited a promising agreement with the numerical results.

Keywords: Contact model, Confined, Compression, Granular materials, Finite element method, Discrete element method

1. Introduction

There is today a strive for an improved mechanistic understanding of powders and granular materials under confined conditions. Such an understanding can be obtained from micromechanical modelling, typically relying on the discrete (or distinct) element method (DEM) [1] (see [2] and references therein). In its usual formulation, the DEM

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uses a simplified contact description, with forces considered to be functions of the particle “overlap”, assuming independent contacts. The assumption of independent contacts is known to limit the applicability of the DEM to moderate strains, corresponding to relative densities up to 0.85–0.90 for nonporous monodisperse spherical particles [3].

One way to overcome this limitation is to mesh each particle by finite elements that enable a superior representation of particle deformation, but also result in a significantly higher computational cost. The thus obtained combined finite/discrete element method (FEM/DEM) [4, 5] is highly valuable to study small particle systems in great detail, but is unpractical for large-scale simulations due to its prohibitive computational cost.

An alternative and interesting approach is to devise more realistic models for the interaction between particles under confined conditions, suitable for implementation in the DEM. Promising advances in this area have been made by Donzé et al. [6, 7], who used volume estimates based on Voronoi constructions in order to enforce the constraint imposed by plastic incompressibility. Aiming mainly at overall global models for powder compression, Montes et al. [8] have introduced the concept of the effective pressure acting on the interparticle contacts, resulting in an interdependence between contacts that again arises from geometric constraints. A nonlocal contact formulation has recently been proposed for confined granular systems where all interactions are assumed to be elastic in nature [9].

Despite this progress, it seems fair to say that confined granular systems are incompletely understood on the micromechanical level. The purpose of this work is to take the first steps towards a mechanistic model for the interaction between plastic particles under confined conditions. Specifically, our aims are, firstly, to identify the determinants of the mechanical response of plastically deforming particles under confined conditions and, secondly, to formulate a simplified analytical model for their interactions.

2. Numerical model and simulations

The finite element method (FEM) was used to study the mechanical response of single particles under triaxial loadings. The onset of plastic flow was governed by the classical von Mises yield function, with yield stress σ_y and no hardening. The elastic response was derived from a free-energy function of the compressible neo-Hookean type, containing two

material constants that for small strains can be identified as the Lamé parameters and calculated from the Young's modulus E and Poisson's ratio ν in the standard manner. The material model used is identical to the one described in Ref. [5] when the latter is specialised to nonporous particles.

Simulations were performed for initially spherical particles with radius $R_0 = 0.5$ mm. The Young's modulus E was kept fixed at 10 GPa, and two different values of Poisson's ratio were used ($\nu = 0.3$ and 0.4), corresponding to bulk moduli $\kappa = E/[3(1 - 2\nu)]$ of 8.33 and 16.67 GPa. Likewise, two different yield stresses were assumed (100 and 200 MPa), corresponding to E/σ_y ratios of 100 and 50. The particles were loaded along the x , y and z directions, using constant loading rates. The loadings will be denoted by $v_x:v_y:v_z$, where v_x , v_y and v_z are loading rates in mm/s. In addition, unconfined uniaxial loadings were also investigated. Due to the reflection symmetries in the x , y and z planes, one octant of the particles was discretised by using about 41 500 hexahedral finite elements and sufficient damping was applied so that quasi-equilibrium was maintained.

3. Formulation of an analytic model

Figure 1: Local contact geometry. The deformed particle shape is described as a truncated sphere of radius R and the distance from the particle centre to contact point i is denoted by r_i .

The key assumptions in the formulation of the analytic model were, firstly, that the deformed particle shape could be approximated by a truncated sphere [8] and, secondly, that the behaviour of each individual contact could be described in terms of a hardness.

From the first key assumption, it follows that each contact surface will be of a circular shape before any impingement of the contacts, with surface area

$$S_i = \pi(R^2 - r_i^2) , \quad (1)$$

where R is the radius of the truncated sphere and r_i is the distance from the centre of the particle to contact point i (Fig. 1). The particle volume can be expressed as

$$V = \frac{4\pi R^3}{3} - \sum_{i=1}^n V_i^{\text{cap}} \quad (2)$$

where

$$V_i^{\text{cap}} = \frac{\pi}{3}(2R^3 - 3R^2 r_i + r_i^3) \quad (3)$$

is the volume of spherical cap i . For simplicity, we will restrict ourselves to small to moderate deformations, so that the above equations remains valid. More general expressions have been published for the case when deformation occurs along three perpendicular directions [8], but these cannot readily be generalised and are therefore not considered further here.

From the second key assumption, it follows that the force exerted on the particle by contact i can be expressed as $\mathbf{F}_i = -HS_i\hat{\mathbf{r}}_i$, where H is a hardness and $\hat{\mathbf{r}}_i$ is a unit vector pointing from the centre of the particle to contact point i . The average stress in the particle can be calculated as [10]

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{i=1}^n \mathbf{F}_i \otimes \mathbf{r}_i \quad (4)$$

where $\mathbf{F}_i \otimes \mathbf{r}_i$ denotes the vector product between $\mathbf{F}_i$ and $\mathbf{r}_i$. Consequently the mean pressure in the particle becomes

$$\bar{P} = -\frac{1}{3} \text{tr } \bar{\boldsymbol{\sigma}} = \frac{\pi H}{3V} \sum_{i=1}^n S_i r_i \quad (5)$$

where $\text{tr } \bar{\boldsymbol{\sigma}}$ indicates the trace of the average stress tensor.

The bulk modulus κ can be interpreted as the ratio between the average pressure $\bar{P}$ and the average volumetric strain $(V_0 - V)/V_0$ (where $V_0 = 4\pi R_0^3/3$ is the initial particle volume) so that the mean pressure can be expressed as

$$\bar{P} = \kappa \left(1 - \frac{V}{V_0} \right) . \quad (6)$$

From the two expressions for $\bar{P}$ embodied in Eqs. (5) and (6), the following consistency condition can be derived

$$\frac{V}{V_0} \left(1 - \frac{V}{V_0} \right) = \frac{H/\kappa}{4R_0^3} \sum_{i=1}^n S_i r_i . \quad (7)$$

The hardness H is generally much smaller than the bulk modulus κ , i.e., $H/\kappa \ll 1$. Hence we obtain

$$\frac{V}{V_0} \approx 1 - \frac{H/\kappa}{4R_0^3} \sum_{i=1}^n S_i r_i , \quad (8)$$

to the first order in H/κ .

By combination of Eqs. (1)–(3) and (8), one obtains a cubic equation in R of the form

$$R^3 - 3AR^2 + 2B = 0 \quad (9)$$

where

$$A = \frac{(3 + H/\kappa) \sum_{i=1}^n r_i}{6(n-2)} , \quad (10)$$

$$B = \frac{4R_0^3 + (1 + H/\kappa) \sum_{i=1}^n r_i^3}{4(n-2)} . \quad (11)$$

The cubic equation (9) can be solved in closed form:

$$R = A \left\{ 2 \cos \left[\frac{\arccos(B/A^3 - 1) + \pi}{3} \right] + 1 \right\} . \quad (12)$$

Once R is found, the magnitude of contact force i is obtained as $F_i = HS_i = H\pi(R^2 - r_i^2)$.

4. Results and discussion

Examples of force–displacement curves for uniaxial and proportional triaxial loading, obtained from FEM simulations, are provided in Fig. 2a ($\nu = 0.3$ and $\sigma_y = 100$ MPa). It is evident that the contact forces are highly dependent on the loading conditions, especially for intermediate and large strains, in agreement with results presented by Donzé et al. [7].

The proportional triaxial loading can serve as an illustration of the mechanical response of the particle under confined conditions. As shown in Fig. 2b, the generic form of the force–displacement curves could be understood as resulting from four sequential deformation stages. First, an initial elastic deformation was observed, consistent with

Figure 2: (a) Examples of force–displacement curves for uniaxial and proportional triaxial loading and (b) deformation stages under confined conditions, as exemplified by proportional triaxial loading ($\nu = 0.3$ and $\sigma_y = 100$ MPa).

the classical Hertzian contact model [11]. Second, local plastic deformation took place in the vicinity of each contact point, as for models of independent contacts [3], yielding a more or less linear increase in force. Third, the coalescence of two or more plastic zones resulted in a reduced stiffness (see below). Fourth, a significantly increased stiffness was seen once the material displaced by plastic deformation started to fill the ambient void space, signifying the onset of a stage dominated by elastic volume reduction of the particle. The dashed line labelled ‘elastic asymptote’ in Fig. 2b was calculated as the product of the asymptotic contact area, $4r^2$, and the asymptotic average pressure, as obtained by

using the asymptotic particle volume, $8r^3$, in Eq. (6). As mentioned, plastic deformation is volume-preserving when a yield condition of the von Mises type is employed, implying that any reduction in particle volume indeed must be of elastic origin. A comparison between Fig. 2a and Fig. 2b indicates that the mechanical response of the particle under unconfined conditions can be understood as resulting from the first three deformation stages.

Insights into the transition between the second and third deformation stage are provided by Johnson’s cavity model [11]. The plastically deformed zone can be approximated as a hemisphere, centred at the contact point, and the hemisphere radius c can be related to the contact force F according to $F = 2\pi\sigma_y c^2/3$ [12]. For uniaxial loading, the plastic zones coalesce when $c = r$. According to Fig. 2a, this occurs at an engineering strain of about 0.1, corresponding to $c = r = 0.45$. For proportional triaxial loading, a straightforward geometrical construction shows that the plastic zones coalesce when $c = r/\sqrt{2}$. In this case, Fig. 2b indicates that coalescence occurs at an engineering strain of about 0.05, corresponding to $r = 0.475$. The forces at coalescence, as obtained from the cavity model, are approximately 42 N for uniaxial loading and 24 N for proportional triaxial loading, in good agreement with the numerical results.

The transition between the third and fourth deformation stage results in a contact pressure that exceeds the hardness. It is interesting to note that a similar, albeit less pronounced effect, has been observed during contact between rough surfaces [13]. For these, a contact pressure exceeding the hardness can be caused by interactions between neighbouring asperities that prevent lateral expansion of the plastic zone [14].

Table 1: Hardness (H) and root-mean-square (RMS) error as obtained from curve fitting.

σ_y (MPa)	ν	H (MPa)	RMS Error (N)
100	0.3	182.2	5.8
100	0.4	183.5	6.1
200	0.3	349.4	9.2
200	0.4	353.4	10.1

Figure 3: Comparison between analytical (lines) and numerical results (symbols) ($\nu = 0.3$ and $\sigma_y = 100$ MPa). The most deformed contacts are represented by solid lines/filled symbols.

We next turn our attention towards the applicability of the analytical model developed in Sec. 3 above. Since the model assumes that the hardness is independent of strain, it cannot capture transition between the second and third deformation stage. By using an average hardness, one can nevertheless obtain a reasonable agreement between analytical and numerical results, as illustrated in Fig. 3 (for $\nu = 0.3$ and $\sigma_y = 100$ MPa). Values of hardness as well as root-mean-square errors over the entire deformation range prior to contact impingement are provided in Table 1 for all investigated combinations of σ_y and ν . As seen, the hardness displays an expected dependence of the yield stress. The transition between the second and third deformation stage became more pronounced with increasing yield stress (data not shown), resulting in somewhat worse agreement between

analytical and numerical results. Overall, the agreement is nevertheless considered to be satisfactory. This is encouraging and indicates that the analytical model could be of practical value. Contrary to the contact models proposed by Donzé et al. [6, 7], our analytical model avoids volume estimates based on Voronoi constructions, which are time-consuming to calculate. However, before the model can be fully utilised in DEM simulations, procedures are needed to handle large strains when contact impingement occurs. In addition, the model could be improved by using a constraint factor that relates the contact pressure to the effective indentation strain.

5. Conclusion

The mechanisms underlying the mechanical response of plastically deforming particles under confined conditions have been identified. An analytical model that exhibits a promising agreement with the numerical results has been formulated.

Acknowledgments

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