Effect of Size Polydispersity on Micromechanical Properties of Static Granular Materials

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Abstract. We analytically investigate the influence of particle size polydispersity on the micromechanical properties of granular packings. In order to approximate the macroscopic quantities in terms of the microscale details, we develop a mean-field approach. It is shown that the trace of the fabric and stress tensors, and the elements of the stiffness tensor can be expressed in terms of dimensionless correction factors (which depend only on the moments of the size distribution), besides the average packing properties such as packing fraction, mean coordination number, and mean normal force. The results of numerical simulations confirm the validity of our analytical predictions, as long as the size distribution is not too wide.

Keywords: polydispersity; granular solids; fabric; micromechanics.
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INTRODUCTION

Size polydispersity is a common property of granular materials in nature and industry, which influences the mechanical behavior and the space-filling properties of such systems [1, 2]. Our goal is to investigate how the macroscopic properties of granular assemblies are affected, when the particle-size distribution deviates from the monodisperse case. The micromechanical approaches, which take the discrete nature of the granular materials into account, are commonly used to describe the behavior. The macroscopic physical properties of the system, e.g. thermal and electrical conductivities and elastic moduli, can be expressed in terms of the microscopic quantities. To examine the sensitivity of these relations, and to estimate the errors when the observable quantities are calculated only from the average packing properties, we develop a mean-field approach to analytically handle the size polidispersity. We have reported the details of analytical calculations and the simulation results in [3]. Here, we aim to clarify the main assumptions, and summarize the most important results.

COORDINATION NUMBER

In order to analytically investigate the influence of size polydispersity on the micromechanical properties of granular materials, we first approximate the coordination number as a function of the particle size and the global mean coordination number of the system. Here, we recall a mean-field approach [4], which has been used to study the properties of the fabric tensor [5]. The method is, however, applicable only to spherical particles. How many contacts, on average, a typical particle of radius r has? To answer this question, one may replace the surrounding random medium of the particle by a homogeneous medium, consisting of particles of average radius $\langle r\rangle$ (as shown in Fig. 1 in a 2D configuration of disks). We denote the particle size distribution by $f(r)$ (with $f(r)dr$ being the normalized probability to find the radius between r and $r+dr$), thus, $\langle r\rangle = \int_0^\infty r f(r)dr$. Each neighboring particle shields the surface of the reference particle, with a shielded area given by $\Omega(r)r$ and $\Omega(r)r^2$, in two and three dimensions, respectively. $\Omega(r)$ is the unit surface angle covered by the neighboring particle:

$$\Omega(r) = \begin{cases} 2\arcsin\left(\frac{\langle r\rangle}{r+\langle r\rangle}\right) & \text{for } D=2 \\ 2\pi\left(1-\frac{\sqrt{(r+\langle r\rangle)^2-\langle r\rangle^2}}{r+\langle r\rangle}\right) & \text{for } D=3 \end{cases}. \tag{1}$$

Taking all neighbors $C(r)$ into account, the total fraction of shielded surface $c_s(r)$ of the reference particle is then given by

$$c_s(r) = \begin{cases} \dfrac{1}{2\pi r}\sum_{i=1}^{C(r)} \Omega(r) r \;= \Omega(r)C(r)/2\pi & \text{for } D=2 \\ \dfrac{1}{4\pi r^2}\sum_{i=1}^{C(r)} \Omega(r) r^2 = \Omega(r)C(r)/4\pi & \text{for } D=3 \end{cases}. \tag{2}$$

Now, we suppose that the total fraction of shielded surface of a particle does not depend on its radius. This is

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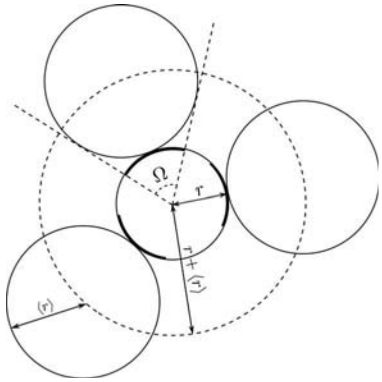

FIGURE 1. A schematic picture depicting the homogeneous surrounding medium of the reference particle with radius r.

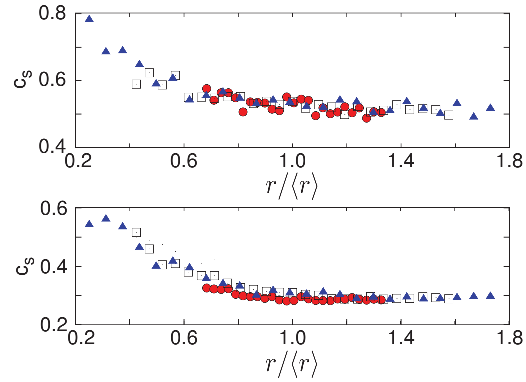

FIGURE 2. The fraction of shielded surface c_s vs. the particle radius r for 2D (top), and 3D (bottom) frictional packings. The different symbols correspond to different types of size polydispersity (see table). The contribution of rattler particles is excluded.

a crucial assumption that makes it possible to estimate $C(r)$. By defining $q_0 = \int_0^\infty f(r)/\Omega(r)dr$, the average coordination number of the packing z becomes

$$z = \int_0^\infty C(r)f(r)dr = \begin{cases} 2\pi c_s q_0 & \text{for } D=2 \\ 4\pi c_s q_0 & \text{for } D=3 \end{cases}. \quad (3)$$

This equation together with Eq. (2) enables us to calculate the coordination number of the particle as a function of its radius as

$$C(r) = \frac{z}{q_0 \Omega(r)}. \quad (4)$$

We perform numerical simulations to investigate the validity of the assumptions made in this section. First, homogeneous packings of particles are generated, by means of the contact dynamics simulation method [6, 7]. The initial dilute configuration of spheres (disks) in a three- (two-) dimensional system with fully periodic boundary conditions is compressed until a static homogeneous packing is constructed. See [8] for the details of the simulation method. The particle radii are uniformly distributed between r_{min} and r_{max}, the friction coefficient is set to 1.0, and there are 10000 and 3000 particles in the system, in $3D$ and $2D$ cases, respectively. In order to study the validity range of our approximations, we construct three different widths of uniform-size polydispersity [9]. The characteristics of these particle size distributions are given in the following table:

symbol	r_{min}	r_{max}	$\frac{r_{max}}{r_{min}}$	$\frac{r_{max}-r_{min}}{2\langle r\rangle}$	$\frac{\langle r^2\rangle}{\langle r\rangle^2}$
•	0.67	1.34	2	0.34	1.04
□	0.40	1.60	4	0.60	1.12
▲	0.22	1.76	8	0.77	1.19

Figure 2 shows the fraction of shielded surface $c_s(r)$ of the particles as a function of their radius. The friction coefficient is set to μ=1.0, and the volume fraction ϕ and average coordination number z of the packings are around $\phi \sim 0.8$ and $z \sim 3.0$, respectively. The covered area Ω_c^p at each contact c of the particle p is calculated according to the radius of the corresponding neighbor. The shielded fraction is then obtained as $c_s^p = \sum_{c=1}^{C_p} \Omega_c^p / 2\pi$ or $c_s^p = \sum_{c=1}^{C_p} \Omega_c^p / 4\pi$ for two- or three-dimensional packings, respectively. The data in Fig. 2 are averaged over particles with radii in the interval $[r, r+\Delta r]$, where Δr is chosen such that we have 25 binning intervals for each data set. We note that the contribution of the rattler particles is excluded in our calculations.

One finds that c_s is approximately constant in r for moderate widths of size distributions. For small particle sizes, however, c_s is noticeably above the average value in wider size distributions. Thus, the small particles are more covered by the neighbors. It has been shown that the situation reverses if rattler particles are included in the calculations [10]. Moreover, upon further compression of the system, the observed deviation decreases as the volume fraction of the packing increases. The value of c_s depends on the dimension of the system and, on the friction coefficient, since increasing the friction reduces the connectivity of the contact network by stabilizing the system in a less dense state. The coordination number $C(r)$, obtained from the simulations, is compared with the analytical estimation of Eq. (4), where the actual size distribution of each numerical packing is used to calculate q_0, z, and $\Omega(r)$ according to Eq. (1). The results are separately shown for two and three dimensions in Fig. 3. While the mean-field approach fits well to the data for moderate size polydispersity, the slopes of the curves be-

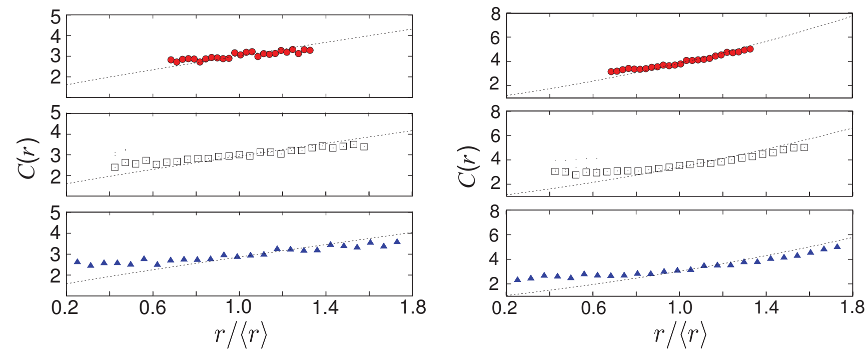

FIGURE 3. Number of contacts $C(r)$ as a function of the particle radius r for 2D (left), and 3D (right) systems from the same data as in Fig. 2. The dashed lines correspond to $C(r)$ according to Eq. (4).

come slightly greater than the corresponding slopes of the fits to the simulation data, when size polydispersity is enhanced. Therefore, one expects that inserting the mean-field value of $C(r)$ would lead to overestimated values for the micromechanical quantities which depend on the contact density.

FABRIC, STRESS, AND STIFFNESS TENSORS

In this section, we briefly explain how the approximations, made in the last section, helps to analytically estimate the macroscopic properties of polydisperse granular materials, when the particle size distribution is given. The results are then compared with the statistics of the numerically generated packings. Let us start with the components of the average fabric tensor, defined as [11]

$$\langle h_{\alpha\beta}\rangle_V = \frac{1}{V}\sum_{p=1}^{N} V_p \sum_{c=1}^{C_p} \frac{l_\alpha^{pc}}{|\vec{l}^{pc}|}\frac{l_\beta^{pc}}{|\vec{l}^{pc}|}, \tag{5}$$

where C_p and V_p are the number of contacts and the volume of particle p, respectively, and $\vec{l}^{pc}$ is the branch vector which connects the center of particle p to its contact c. The trace of the fabric tensor in the continuum limit (assuming a polydisperse distribution of particle radii $f(r)$) is given by

$$\langle h_{\alpha\alpha}\rangle_V = \frac{N}{V}\int_0^\infty V(r)C(r)f(r)dr. \tag{6}$$

Replacing the coordination number from Eq. (4), one finds [3]

$$\langle h_{\alpha\alpha}\rangle_V = \phi z g_1, \tag{7}$$

where ϕ is the packing fraction, and the correction factor g_1 is defined as

$$g_1 = \frac{\int_0^\infty V(r)\frac{f(r)}{\Omega(r)}da}{q_0\int_0^\infty V(r)f(r)dr} = \begin{cases} \frac{\langle r^2\rangle_g}{\langle r^2\rangle} & \text{for } D=2 \\ \frac{\langle r^3\rangle_g}{\langle r^3\rangle} & \text{for } D=3 \end{cases}, \tag{8}$$

with $\langle r^n\rangle$ denoting the n-th moment of the size distribution $f(r)$, and $\langle r^n\rangle_g$ similarly for the modified distribution $f(r)/\Omega(r)$ normalized by q_0. Importantly, one only needs the size distribution $f(r)$ to calculate g_1.

Next we turn to the micromechanical expressions for the components of the average stress tensor $\langle\sigma_{\alpha\beta}\rangle_V$ of a static granular assembly

$$\langle\sigma_{\alpha\beta}\rangle_V = \frac{1}{V}\sum_{p=1}^{N}\sum_{c=1}^{C_p} l_\alpha^{pc} F_\beta^{pc}. \tag{9}$$

Here, $\vec{F}^{pc}$ is the contact force exerted on particle p by its neighboring particle at contact c. Assuming an average normal force $\bar{F}_n^p$ around the particle p which depends on the particle size, the continuous limit of Eq. (9) for the trace of the average stress tensor is given by

$$\langle\widetilde{\sigma}_{\alpha\alpha}\rangle_V = \frac{N}{V}\int_0^\infty r\bar{F}_n(r)C(r)f(r)dr, \tag{10}$$

and if one further assumes that the contact force exerted on a particle increases with increasing the radius, so that the $\bar{F}_n(r)/C(r)$ remains roughly constant [12], after some calculations one gets

$$\langle\widetilde{\sigma}_{\alpha\alpha}\rangle_V = \frac{\phi z\,\bar{F}_n(\langle r\rangle)\,g_2}{\pi} \times \begin{cases} 1/\langle r\rangle & \text{for } D=2 \\ 3/4\langle r^2\rangle & \text{for } D=3 \end{cases}, \tag{11}$$

with

$$g_2 = \frac{\pi\int_0^\infty r\frac{f(r)}{\Omega^2(r)}dr}{q_0} \times \begin{cases} \langle r\rangle/3\langle r^2\rangle & \text{for } D=2 \\ (2-\sqrt{3})\,\langle r^2\rangle/\langle r^3\rangle & \text{for } D=3 \end{cases}. \tag{12}$$

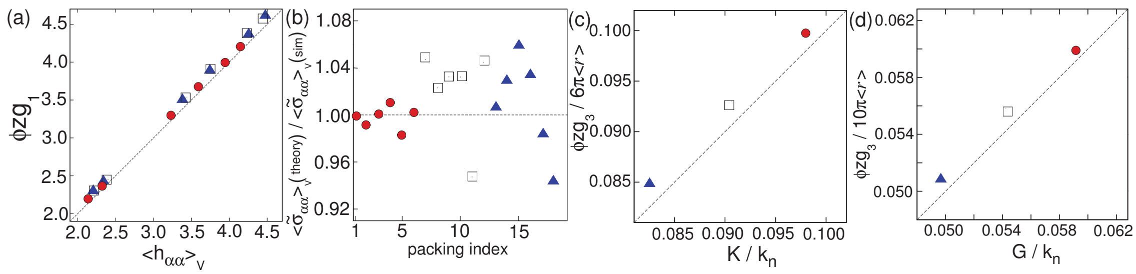

FIGURE 4. The estimated value compared with the exact result (obtained from the simulations) for (a) the trace of the average fabric tensor, (b) the trace of the stress tensor, (c) the bulk modulus, and (d) the shear modulus. Each data point corresponds to a different 3D frictionless packing. The same symbols as in Fig. 2 are used.

Finally, we study the influence of polydispersity on the elements of the stiffness tensor, which described the linear response of a material to small deformations. The integral form of the volume weighted average of the 4th rank stiffness tensor (assuming a polydisperse probability distribution) is given by [13]

$$\langle C_{\alpha,\beta,\gamma,\eta}\rangle_V = \frac{Nk_n}{V}\int_0^\infty 2r^2\left(\sum_{c=1}^{C(r)} n_\alpha^c n_\beta^c n_\gamma^c n_\eta^c\right) f(r)dr. \tag{13}$$

where $\hat{n}^{pc}$ is the normal unit vector at contact c, and k_n is the normal spring constant. This equation is only valid for the case of frictionless packings ($k_t = 0$). For the general case of frictional systems, see [3]. One can find the elements of the stiffness tensor of an isotropic packing and, after some calculations, it is possible to present the macroscopic elastic properties such as the shear G and bulk moduli K in terms of the average packing properties and the correction factor g_3:

$$G/k_n = (\phi z g_3)/(10\pi\langle r\rangle), \tag{14}$$

and

$$K/k_n = (\phi z g_3)/(6\pi\langle r\rangle). \tag{15}$$

The correction factor g_3 is defined as

$$g_3 = \begin{cases} \langle r^2\rangle_g/\langle r^2\rangle & \text{for } D=2 \\ \langle r\rangle\langle r^2\rangle_g/\langle r^3\rangle & \text{for } D=3 \end{cases}. \tag{16}$$

We note that in the limit of narrow size distributions, one can purely express g_i factors in terms of the moments of the size distribution function $f(r)$. In Fig. 4, we present the exact values of the desired quantities obtained from the simulations versus the analytical predictions (using the average properties of the numerical packings, wherever needed). The agreement is satisfactory, providing that the particle-size distribution is not too wide. To conclude, we have shown that knowing the functional form of the (moderate) size polydispersity, together with the average packing properties, would be enough to determine the micromechanical properties within a reasonable error margin.

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