

Experimental and DEM assessment of stress-dependency of surface roughness effect on sample shear modulus

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Abstract:

This contribution assesses the effect of particle surface roughness on the shear wave velocity V_S and the small-strain stiffness of soils G_0 using both laboratory shear plate dynamic tests and discrete element method (DEM) analyses. Roughness is both controlled and quantified to develop a more comprehensive understanding than was achieved in prior contributions that have involved binary comparisons of rough and smooth particles. Glass beads were tested to isolate surface roughness effects from other shape effects. V_S and G_0 were accurately determined using a new design configuration of piezo-ceramic shear plates. Both the experimental and DEM results show that increasing surface roughness reduces G_0 particularly at low stress levels; however, the effect is less marked at high pressures. For the roughest particles, Hertzian theory does not describe the contact behaviour even at high pressures; this contributes to the fact that the exponent in the G_0 – mean effective stress relationship exceeds 0.33 for sand particles. Particle-scale analyses show that the pressure-dependency of surface roughness effects on G_0 can be interpreted using a roughness index α which enables the extent of the reduction in G_0 due to surface roughness to be estimated.

Introduction

Soils are granular materials consisting of many particles, and the overall response of a soil can be considered to be a complex accumulation of the inter-particle responses. The inter-particle responses can be directly affected by particle characteristics such as surface roughness; however, our understanding of the link is incomplete.

Accurate knowledge of soil stiffness is important to predict ground deformation during construction as it directly relates the applied stress to the strain and hence the displacement of the ground (Atkinson 2000; Clayton 2011). It is well known that the small-strain shear modulus G_0 is influenced by effective confining pressure p' and void ratio e , and is often expressed as $G_0 = AF(e)p'^n$ where A and n are material constants and $F(e)$ is a void ratio function for G_0 . The material constant n that describes the stress-dependency of the soil is often approximated to be 0.5 for sands. From a micromechanical perspective, n is related directly to the response at grain contacts, and n can be influenced by presence of surface asperities (Goddard 1990; Yimsiri & Soga, 2000).

Experimental assessments of surface roughness effects on G_0 have rarely been reported in the literature most likely due to limitations associated with accurately measuring and controlling surface roughness. Santamarina & Cascante (1998), Sharifipour & Dano (2006) and Otsubo et al. (2015) observed a reduced shear wave velocity (V_s), and thus G_0 , for roughened spherical materials. The sensitivity of the overall behaviour to the degree of roughness was not ascertained as in each case only one level of roughness was compared with a smooth reference case.

Discrete element method (DEM) studies enable a systematic investigation of surface roughness effects. Cavarretta et al. (2010) developed a rough contact model based on their particle-scale compression tests; this model, whose input parameters include both surface roughness and hardness, was implemented in a DEM code by O'Donovan et al. (2015). Developing these ideas, and drawing on fundamental tribology research, Otsubo et al. (2017) proposed an alternative contact model that does not include hardness as a model parameter.

Surface topographies of sand grains can now be measured accurately using white light interferometry (e.g. Cavarretta et al., 2010; Altuhafi & Coop, 2011). In this contribution the surface roughness of spherical particles was systematically varied and measured to advance understanding of how the degree of roughness influences overall behaviour of soils. Glass beads (ballotini) with four surface roughness values were tested in this study. While the use of ballotini limits direct, quantitative application of the findings to real soils consisted of angular grains, a fundamental understanding of the effect of surface roughness on G_0 can be developed. Following Brignoli et al. (1996) piezo-ceramic shear plates were used to measure V_s . Equivalent DEM simulations were performed to provide additional insight into particle-scale response.

Experimental Procedure

Test materials

The borosilicate glass ballotini used in the laboratory experiments had a mean particle diameter $\bar{D} = 1.2$ mm ($1 \leq D \leq 1.4$ mm) (Table 1). The as-supplied smooth ballotini (Fig. 1(a)) were processed to increase the surface roughness by milling 30 g of the ballotini and 15 g of Toyoura sand (as-supplied) in a glass jar for 0.5, 5 and 25 hours as detailed in Cavarretta et al. (2012), and they were separated using a sieve with 0.85 mm openings. Representative microscopic images and surface topographies of roughened ballotini produced are illustrated in Fig. 1. Root mean square (RMS) surface roughness S_q , skewness S_{sk} , and kurtosis S_{ku} values were measured using a Fogale Microsurf 3D optical interferometer and quantified as:

$$S_q = \sqrt{\frac{1}{m} \sum_{i=1}^m Z_i^2} \quad (1a)$$

$$S_{sk} = \frac{1}{mS_q^3} \sum_{i=1}^m Z_i^3 \quad (1b)$$

$$S_{ku} = \frac{1}{mS_q^4} \sum_{i=1}^m Z_i^4 \quad (1c)$$

where m = number of discrete data points; and Z_i = elevation relative to the reference surface. The reference surface is not planar for soil grains, and the effect of curvature should be removed from as-measured data (Otsubo et al., 2014). Yang et al. (2016) proposed use of a fractal dimension to characterise the surface roughness; however, here a motif analysis algorithm implemented in the Fogale 3D Viewer software (Fogale, 2005) was used to remove the curvature effects adopting a shape motif size of 17.5 μm of the side length of a square considered (70 μm). The surface roughness values stated are the average of 40 measurements on each type of particle; in each case 10 particles were considered and the measurements were taken at four different locations on each particle. The variations of measured surface roughness parameters with their mean values are illustrated in Fig. 2 considering both the flattened and non-flattened (as-measured) surfaces. Both S_{sk} and S_{ku} exhibit considerable scattering for smoother cases. Referring to Fig. 2c, large values of S_{ku} are not shown; their maximum value and standard deviation are provided in Table 2. In contrast, measurable differences are confirmed in S_q , and thus S_q is used as a representative roughness parameter in the following discussions. The four surface types with $S_q = 58, 127, 267$ and 586 nm are referred here to as Lab-58, Lab-127, Lab-267 and Lab-586, respectively. The shape of the ballotini before and after milling for 25 hours were quantified using a Qicpic image analysis sensor (Witt et al. 2004; Altuhafi & Coop 2011), and both cases showed sphericity = 0.94, aspect ratio = 0.96 and convexity = 0.99, indicating that the overall shape was not affected by the milling process.

The minimum and maximum void ratios (e_{min} and e_{max}) for each surface type were measured following the JGS standard (JGS 0161, 2009) as listed in Table 1 and illustrated in Fig. 3. The maximum particle diameter tested ($D_{max} = 1.4$ mm) is large relative to the standard container (40 mm high and 60 mm wide); a larger container 64.3 mm in height and 79.9 mm in diameter was used. Referring to Fig. 3, both e_{min} and e_{max} increase with increasing S_q non-linearly; an increase in S_q has a negligible effect on the extreme void ratios for S_q values > 250 nm.

Sample preparation

Cylindrical specimens (≈ 110 mm high and ≈ 50 mm wide) composed of the four surface types of ballotini were tested in a triaxial apparatus. The four specimens were prepared with a target void ratio $e_{target} \approx 0.6$. For the smooth surface ballotini ($S_q = 58$ nm), e_{target} was achieved by slowly pluviating the ballotini into a metal mold using a funnel keeping the tip of the funnel just above the rising sample surface. The rough ballotini sample ($S_q = 586$ nm) was prepared by dividing the sample volume into 10 layers, and tapping the side wall with a metal bar. A consistent number of blows was applied to each layer to achieve uniform densification. After placing a topcap on the sample, a vacuum (negative) pressure of 30 kPa was applied before dismantling the mold. The e values measured at $p' = 30$ kPa of vacuum pressure are noted as the initial void ratio (e_0) in Table 1.

Dry samples were tested. To measure the variation in the sample dimensions during the isotropic compression, two axial displacement sensors each 50 mm long and a radial displacement sensor were placed at the mid-height of the sample. Only isotropic compression was considered and the topcap of the sample was not fixed to a loading rod. The mass of the topcap added a vertical pressure of 1.5 kPa to the sample. No porous stone was placed so that the sample contacted the shear plates directly. Confinement was achieved by supplying air pressure to the cell to maintain the sample dry. The pressure levels considered were $p' = 50, 100, 200, 400, 750$ and 1500 kPa; additional finer pressure increments were considered for the rougher ballotini samples. For the sample with $S_q = 127$ nm the maximum pressure tested was $p' = 750$ kPa.

Shear plate dynamic tests

Previous researchers including Brignoli et al. (1996), Ismail & Rammah (2005) and Suwal & Kuwano (2013) have emphasized that because shear plates are embedded into the topcap and base pedestal the sample fabric is not disturbed compared with the case where bender elements are used (Fig. 4(a)). Brignoli et al. (1996) and Ismail & Rammah (2005) compared bender element and shear plate signals and found better signals with shear plates for coarse sands particularly at high pressure environment. The DEM simulations by O'Donovan (2013) indicate that where the particle size is finite relative to the bender element size, the bender element signals are sensitive to local packing effects (Fig. 4(b)). Consequently this study developed a new shear plate configuration comprised of two rectangle shear plate elements (PZT505), manufactured by Morgan Advanced Materials. Each plate had dimensions $15 \times 30 \times 1$ mm (Fig. 5(a)). The elements comprise lead zirconate titanate (PZT) with material density = 7800 kg/m^3 and Poisson's ratio = 0.3. The planar piezo-electric element converts an applied force to an electric signal, and vice versa, and it operates in shearing mode. The two transmitter elements were wired in parallel so that they received the same applied voltage and have identical deformation. The two elements on the topcap were excited together, and the signals received at two elements on the pedestal were summed to interpret the signals (Otsubo, 2016).

The test procedure, schematically shown in Fig. 5(b), is similar to that for a conventional bender element test. An inserted electric (voltage) signal was specified using a function generator to control the shear plate movement. The inserted and received signals were recorded using two oscilloscopes each having two channels.

The recorded signals were averaged over 4 to 128 signals to reduce background noise. Two custom-made amplifiers were used to amplify the received signals by a factor of 100. The sinusoidal pulse inserted to the sample had a voltage amplitude of ± 10 V with inserted frequencies f_{in} ranged from 5 to 40 kHz. A creep time was allowed for each sample to reach equilibrium when no increase in V_S with time was measured. The creep time allowed was determined empirically, at least 1 hour for the smooth ballottini samples and 2 hours for the roughened ballottini samples.

DEM simulation method

The DEM simulations used the contact model for rough surfaces proposed in Otsubo et al. (2017) that captures the asperity-dominated response at low normal contact force (N) without modifying the geometry of spheres. The model is detailed in Otsubo et al. (2017) and Otsubo (2016) and key features are summarized here for completeness. The following material properties of ballottini were considered: particle density $\rho_p = 2600$ kg/m³, particle Young's modulus $E_p = 70$ GPa, and particle Poisson's ratio $\nu_p = 0.2$. According to the manufacturer's data sheets the ballottini had $E_p = 77$ GPa, however Caverretta et al. (2012) reported slightly lowered E_p values for similar ballottini compared based on particle compression tests. The lower E_p value measured can be explained by imperfections in the manufactured product. The present study used a reduced $E_p = 70$ GPa with a typical value of $\nu_p = 0.2$. Effective medium theory gives a relationship $G_0 \propto E_p^{2/3}$ (Yimsiri & Soga, 2000). Referring to Fig. 6, the model considers three types of behaviour: asperity dominated (Eq. 2), a transitional behaviour (Eq. 3) and Hertzian (elastic) behaviour (Eq. 4). The behaviour type depends on the contact overlap δ relative to the combined surface roughness S_q^* :

$$N = N_{T1} \left(\frac{\delta}{2.11 S_q^*} \right)^{2.59} \quad \delta < 2.11 S_q^* \quad (2)$$

$$N = N_{T2} \left(\frac{\delta - 0.82 S_q^*}{23.65 S_q^*} \right)^{1.58} \quad 2.11 S_q^* \leq \delta < 24.47 S_q^* \quad (3)$$

$$N = \frac{4}{3} E_p^* R^{*0.5} (\delta - 2.06 S_q^*)^{1.5} \quad 24.47 S_q^* \leq \delta \quad (4)$$

where $1/R^* = 1/R_1 + 1/R_2$, $1/E_p^* = (1 - \nu_{p,1}^2)/E_{p,1} + (1 - \nu_{p,2}^2)/E_{p,2}$, $S_q^{*2} = S_{q,1}^2 + S_{q,2}^2$ where the subscripts 1 and 2 correspond to the properties of two particles in contact;

$$N_{T1} = S_q^* E_p^* \sqrt{2 R^* S_q^*} \quad (5)$$

and $N_{T2} = 100 N_{T1}$.

For perfectly smooth surfaces, substituting $S_q^* = 0$ into Eq. 4 reduces the rough contact model to the Hertzian contact, given by:

$$N = \frac{4}{3} E_p^* R^{*0.5} \delta^{1.5} \quad (6)$$

The normal contact stiffness k_N can be obtained by differentiating N in Eqs. 2 to 4 with respect to δ , and the tangential contact stiffness k_T is related to k_N as in a simplified Hertz-Mindlin contact model to give:

$$k_T = \frac{2(1 - \bar{\nu}_p)}{2 - \nu_p} k_N \quad (7)$$

where $\bar{\nu}_p = (\nu_{p,1} + \nu_{p,2})/2$. The tangential contact force T is updated in an incremental manner subject to an upper limit that $T = \mu N$. Eq. 7 assumes zero tangential movement at contacts; a more sophisticated approach considering partial slip is discussed in O'Donovan et al (2015) and Otsubo (2016).

The DEM simulation approach is similar to that adopted by Otsubo et al. (2017) and a modified version of the LAMMPS molecular dynamics code (Plimpton, 1995) was used. Referring to Fig. 7, rectangular samples with lateral periodic boundaries in the X and Y directions and rigid wall boundaries in the Z direction were used. The particle material properties were assigned to the wall boundaries. The samples were formed of 155,165 spheres (height, $L \approx 100$ mm and width ≈ 50 mm). The particle diameters correspond to the tested ballotini. To prepare DEM samples, non-contacting particles were initially generated, and an isotropic compression was applied using a servo-control algorithm. The inter-particle friction used during the isotropic compression μ_{prep} was set to be 0.1. The simulations here did not include a gravitational force. Viscous damping was activated after $p' = 1$ kPa was achieved to remove kinetic energy of vibrating particles, and the damping was kept active during the subsequent compression to target stresses. The viscous damping was turned off during wave propagation simulations. The inter-particle friction during wave propagation simulations μ_{wave} was increased to 0.2 from μ_{prep} to ensure elastic response at contacts (i.e. slip at tangential contact is avoided (Otsubo, 2016)).

Five samples with differing roughness values were prepared: $S_q = 0, 70, 140, 280$ and 600 nm, the e_0 and mean coordination number $\bar{C}_N$ (number of contacts per particle) values at $p' = 25$ kPa are shown in Table 3. Stress wave propagation simulations were performed at $p' = 50, 100, 200, 400, 800$ and 1600 kPa.

The entire bottom wall (transmitter wall) was perturbed in a transverse (X-) direction to generate S-waves that propagated in the longitudinal (Z-) direction. The wall movement was a sinusoidal pulse with a phase delay of 270 degrees, double amplitude $2A = 5$ nm and various f_{in} as considered in the laboratory tests (Fig. 7(b)). The stress responses at the transmitter and receiver walls were recorded; the resultant shape of the stress response at the transmitter was almost a sinusoidal pulse without a phase delay as shown below (Fig. 9(b)).

Void ratio correction

A void ratio correction $f(e)$ was applied to isolate the effect of void ratio on the shear wave velocity V_s . Following Hardin & Richart (1963) a linear correlation was assumed such that:

$$f(e) = B - e \quad (8)$$

where B is determined from V_S measurements on samples with different e values. Ideally, several pressure levels should be considered to obtain $f(e)$ with confidence; however, this study considered only $p' = 50$ kPa under a vacuum pressure. For the surface types with $S_q = 58, 127$, and 586 nm various samples were prepared with differing varying e values. The same batch of materials were used repeatedly for the test series and so care was taken not to increase p' larger than the test pressure ($p' = 50$ kPa) to avoid yielding of the asperities which might modify the contact behaviour. The test results showed no measurable effects of using the same materials repeatedly.

This study used the peak-to-peak method in which the time delay between first peaks of inserted and received signals is taken as the travel time T_{travel} , and so $V_S = L/T_{travel}$. Using DEM simulation data, Otsubo et al. (2017) showed that provided the signal quality is good, e.g. planar wave propagation with a periodic system, the peak-to-peak method gives accurate V_S compared to a direct measurement of waves propagating through the system. However, this ideal condition cannot be achieved in the experiments. Consequently, following Yamashita et al. (2009) f_{in} was adjusted to a dominant frequency in the received signals to minimize the difference in V_S between the peak-to-peak method and the start-to-start method. Thus, $f_{in} = 7$ kHz was considered for the smooth case ($S_q = 58$ nm), while $f_{in} = 5$ kHz was selected for rougher cases ($S_q = 127$ and 586 nm). The variation in V_S with e at $p' = 50$ kPa for the three surface types are illustrated in Fig. 8; at a given void ratio V_S decreases systematically with increasing roughness. Straight lines with $B = 1.28$ give a good fit to most of the data. The discrepancy for the two data points obtained for $S_q = 127$ nm at low e values highlights the limitation of applying a simple linear fitting. However, the e values of the samples with $S_q = 127$ nm considered below all exceed 0.594 and so this study applies $B = 1.28$ in Eq. 8. The B value obtained here is smaller than that reported in sands (e.g. $B = 2.17$, Hardin & Richart (1963)). Otsubo (2016) obtained $B = 1.19$ to 1.48 for monodisperse spheres using DEM where the difference depends on consideration of the volume of rattler particles (with $C_N = 0$ or 1) that do not carry forces. Xu et al. (2013) reported $B = 1.16$ for slightly polydisperse spheres based on their DEM simulations. Thus $B = 1.28$ was also applied to analyse DEM results.

Stress-dependent dynamic sample response

The time domain responses of experimental and DEM samples for smooth and medium rough surface cases for $f_{in} = 10$ kHz are illustrated in Figs. 9(a) and (b), respectively, for three pressure levels. The horizontal axis is normalised by the sample length L at each pressure level, and vertical axis is normalised by their maximal amplitudes over the duration. These signals are still affected by void ratio and so a direct comparison cannot be made between the laboratory and DEM data. The smooth case clearly exhibits the shortest travel time for both experimental and DEM data at $p' = 50$ kPa. The difference in the arrival time between the smooth and rough cases becomes less obvious as pressure increases, and the overall shape of the signals becomes similar. The shear stress recorded on the boundary walls in X-direction in the DEM samples is more coherent with a

clear sinusoidal shape when compared with the laboratory data. Experimental data show significant dispersion of waves with time in which experimental signals include reflections at the side boundary, while more coherent waves are observed in the DEM samples where an ideal periodic boundary condition is applied.

Prior research has shown that additional insight into the sample and material properties can be attained via frequency domain analysis (e.g. Santamarina & Aloufi, 1999; Greening & Nash, 2004; Alvarado & Coop, 2012). The frequency domain responses of the specimens at the lowest and the highest pressures are shown in Fig. 10 by considering the gain factor (received FFT amplitude / inserted FFT amplitude). These data were generated by firstly confirming that the gain factor at a given frequency is insensitive to the nominal frequency of the input signal (f_{in}), and then f_{in} values were varied to obtain gain factor data for the widest possible range of frequencies. The maximum gain factor for the DEM samples exceeds 1 due to the absence of viscous or local damping, and the fixed receiver wall that stored more strain energy compared with the transmitter wall.

The variation in gain factor with frequency differs between the laboratory and DEM data. The laboratory data exhibits anti-resonant behaviour at around 12 kHz and 22 kHz for the samples confined at 50 kPa and 1500 kPa, respectively, and this may have been induced by the waves reflected at the lateral boundaries as reported in Arroyo et al. (2006). DEM data do not include such a behaviour due to the lateral periodic boundaries. It is the range of frequencies that are more interesting as the maximum transmissible frequency ($f_{low-pass}$) is a function of the granular material. For both sample types $f_{low-pass}$ decreases with increasing surface roughness and increases with increasing p' . A systematic variation in $f_{low-pass}$ with S_q is most evident in the DEM data at $p' = 50$ kPa. At $p' = 1500$ kPa the DEM samples have $f_{low-pass}$ values between about 52 and 55 kHz. For the laboratory samples, the relative difference in the $f_{low-pass}$ values is smaller at $p' = 1500$ kPa in comparison with $p' = 50$ kPa. The broader variation in the $f_{low-pass}$ values in the experiments in comparison with the simulations may be a result of the range of roughness values that inevitably exist in the physical samples. The dependency of $f_{low-pass}$ on both p' and surface roughness reflects a dependency of $f_{low-pass}$ on the contact stiffness.

Dynamic sample shear modulus

The V_s data were used to determine G_0 assuming the material to be isotropic and homogeneous as:

$$G_0 = \frac{\rho_p}{1+e} V_s^2 \quad (9)$$

As noted above, the dependency of G_0 on e and p' is often expressed as:

$$G_0 = AF(e) p'^n \quad (10)$$

Developing on Eqs. 8-10 with $B = 1.28$ gives:

$$F(e) = \frac{(1.28 - e)^2}{1 + e} \quad (11)$$

To isolate the effect of e , experimental and DEM data showing the variation in $G_0/F(e)$ with p' are given in Figs. 11(a) and (b), respectively. In both cases, at a given p' , $G_0/F(e)$ decreases with increasing S_q ; the extent of the variation decreases with increasing pressure. The data for roughened ballotini approach the smooth equivalent in both the laboratory and DEM cases at high pressures. The exponential slopes n in Eq. 10 obtained for each sample type considering all the pressure levels are illustrated in Fig. 12(a) with reference slopes $n = 1/3$ and $1/2$, and it is clear that n increases with increasing S_q . For all the cases n value exceeds $1/3$ predicted from Hertzian theory (for a stable lattice packing) and for roughened ballotini samples n approaches the value of 0.5 typically associated with sands (McDowell & Bolton, 2001). The slopes were obtained considering all the pressure levels; however, n for roughened ballotini becomes larger if the data for low pressures only are considered, whereas n decreases for consideration of high pressures only. The relationship between the exponential slopes n and the material constant A (Eq. 10) follows a trend in which the larger the n value becomes the lower the A value becomes (Fig. 12(b)); this observation is also noted in Sharifipour & Dano (2006).

For DEM samples, the link between $G_0/F(e)$ and the normal contact stiffness k_N was investigated. Fig. 13 illustrates a linear relationship between $G_{0,DEM}^{rough} / G_{0,DEM}^{smooth}$ and $k_{N,DEM}^{rough} / k_{N,DEM}^{smooth}$ averaged over all the contacts in each sample, where the superscript smooth corresponds to the DEM sample with $S_q = 0$ (Dem-0) at identical pressure levels. The linear trend observed between the overall sample stiffness and the contact stiffness, for a given particle size distribution, agrees with micromechanical effective medium theory as analysed by Yimsiri & Soga (2000). The reduction in G_0 due to surface roughness is caused by the reduction in the inter-particle stiffness affected by the presence of asperities.

Considering the DEM data, it is interesting to quantify the relative proportions of the contact behaviour types (Fig. 6) for the samples with non-zero S_q values. Referring to Fig. 14 in all cases, a negligible proportion of contacts exhibits Hertzian behaviour; the proportion is finite only for $S_q = 70$ nm at $p' = 1600$ kPa and even in this case only 30% of the contacts can be considered Hertzian. For the samples with $S_q \geq 140$ nm, asperity contacts dominate at low pressures, and the contact behaviour becomes transitional as the pressure increases.

To enable comparison between experimental and DEM data, $G_0/F(e)$ values for the laboratory and DEM data were normalised by that for DEM sample ($G_{0,DEM}^{smooth}/F(e)$). Fig. 15 illustrates the relationship between $G_0/F(e)$ normalised by $G_{0,DEM}^{smooth}/F(e)$ and $\bar{S}_q$ normalised by the mean particle radius, $\bar{R}$ ($= 0.6$ mm) at two pressure levels. There is a systematic monotonic reduction in G_0 with S_q at both low and high pressures; the sensitivity of G_0 to S_q is reduced at larger S_q . For the laboratory data at $p' = 750$ kPa no significant reduction in G_0 is observed between $S_q = 267$ and 586 nm, the DEM data indicate a slightly greater dependency of G_0 on S_q . The $G_0/F(e)$ values for the laboratory samples are reduced by 50% compared with the equivalent smooth case at $p' = 50$ kPa; DEM data indicate a slightly greater reduction. In contrast, at the higher pressures $p' = 750 - 800$ kPa, the reduction in G_0 is less marked (at most 20%) in both cases.

Application of roughness index

The stress- and roughness-dependency of the small-strain shear modulus highlighted can be accounted for by using a particle-scale roughness index α (Greenwood et al. (1984)), given by:

$$\alpha = \frac{S_q^*}{\delta^{smooth}} \quad (12)$$

where δ^{smooth} = equivalent overlap for a smooth contact at a given normal contact force N , i.e. δ^{smooth} accounts for variations in pressure. Rearranging Eq. 6 for Hertzian (smooth) contacts gives:

$$\delta^{smooth} = \left[\frac{3}{4} \frac{N}{E_p^* R^{*0.5}} \right]^{2/3} \quad (13)$$

Substituting N obtained from Eqs. 2 to 4 into Eq. 13 and then Eq. 12 enables estimation of α for rough contacts in which N can be directly extracted from the DEM datasets. An estimate of the mean normal contact force for the laboratory samples was made by applying effective medium theory (Chang et al., 1991):

$$\bar{N} = \frac{4\pi \bar{R}^2 (1+e)}{\bar{C}_N} p, \quad (14)$$

For the laboratory samples, the mean coordination number, $\bar{C}_N$, cannot be easily obtained. Using the same type of ballotini with D ranged from 1 and 1.18 mm, Otsubo (2016) measured $\bar{C}_N$ based on both laboratory tests and DEM simulations. The laboratory tests include the ink tests (Bernal & Mason, 1960; Oda, 1977) and μ CT scanning using both the smooth and rough surface ballotini as used in this study. The laboratory and DEM data for the $\bar{C}_N - e$ relationship presented in Otsubo (2016) are captured by analytical expressions proposed by Nakagaki & Sunada (1968) and Suzuki et al. (1981), respectively, for the range of void ratios considered in this study. Considering the variation in the $\bar{C}_N - e$ relationship, $\bar{C}_N$ data obtained using both analytical expressions were considered in this study, i.e. two values of $\bar{N}$ were estimated from two $\bar{C}_N$ values for each sample. As the result, two α values were found for each sample using Eqs. 12 and 13.

Figure 16(a) illustrates the variation in $G_0^{rough} / G_{0,DEM}^{smooth}$ correlated with α for all the test cases where the laboratory data have a range of α for each sample as described above. For the DEM samples, $G_0^{rough} / G_{0,DEM}^{smooth}$ systematically decreases with increasing α , the trend can be captured by the expression $G_0^{rough} / G_{0,DEM}^{smooth} = 0.0211\alpha^2 - 0.211\alpha + 0.967$ with a coefficient of determination 0.997. While the laboratory data points exhibit a similar trend there is more scatter, the most noticeable difference between the laboratory and DEM data is for $\alpha > 1.5$ where the DEM data clearly predict a greater reduction in the sample stiffness than the laboratory data.

A possible explanation for the differences at higher α values is given in the origin of the contact model. The model was developed by considering particle-scale experimental data of Greenwood et al. (1984) and an

analytical expression by Yimsiri & Soga (2000) (Fig. 16(b)). Greenwood et al. (1984) measured the radius of contact area for both smooth and rough contacts; however, their test data are limited up to $\alpha \approx 1$ (Fig. 16(b)). Referring to Fig. 16(a), a good correlation between G_0 and α is observed for both experiments and DEM up to $\alpha \approx 1$.

The data shown in Fig. 14 are revisited using α in Fig. 17 for all the DEM data points where the inset figure shows the variations for low α values. Hertzian contact behaviour dominates at $\alpha < 0.04$, transitional contacts are in the majority at $0.04 \leq \alpha < 1$, and asperity contacts are dominant at $\alpha > 1$. Greenwood et al. (1984) concluded that a rough contact with $\alpha < 0.05$ can be approximated to be a Hertzian contact with an error of less than 7%, and this agrees with the results presented in Fig. 16(a).

Conclusions

This contribution has assessed the influence of particle surface roughness on the small-strain shear modulus G_0 of ballotini samples. Surface roughness was controlled and measured, and a range of roughness values were considered to discuss roughness-dependency of G_0 . Piezo-ceramic shear plate dynamic tests were carried out and supplemental DEM analyses provided additional insight as below:

- For equivalent particles at lower roughness values an increase in surface roughness increases both e_{min} and e_{max} ; however, there is a threshold roughness value beyond which further increases in roughness do not increase e_{min} or e_{max} .
- The shear wave velocity and thus G_0 decrease with increasing S_q value in a non-linear manner, and the difference in G_0 reduces as the confining pressure (p') increases. The low-pass frequency limit ($f_{low-pass}$) decreases with increasing S_q ; $f_{low-pass}$ increases with increasing p' and the sensitivity to initial roughness decreases with increasing p' .
- The reduction in G_0 can be well correlated with a reduction in the inter-particle stiffness affected by surface asperities. At low p' , interaction between asperities governs the overall sample response.
- The exponential constant n in the $G_0 - p'$ relationship increases with increasing S_q with n being greater than $1/3$ derived from Hertzian theory and approaching 0.5 obtained typically for sands.
- Particle-scale analyses indicate that Hertzian contacts are rarely observed for rough contacts even at higher p' , and this explains partially that $n = 1/3$ is not observed for sands with a finite surface roughness.
- The roughness effects on G_0 depend highly on p' , resulting in a complex relationship between G_0 and S_q .
- A roughness index α can be well correlated with a reduction in G_0 for $\alpha < 1$, which agrees with the literature. Thus the reduction in G_0 due to surface roughness can be predicted from contact overlap data available in a DEM sample.

- However, for $\alpha > 1$ where the overall behaviour is dominated by response of asperities, the current contact model for rough surfaces needs to be validated against more fundamental particle-scale experiments.

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