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Effect of sample size on the response of DEM samples with a realistic grading

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Abstract This paper shows that for DEM simulations of triaxial tests using samples with a grading that is representative of a real soil, the sample size significantly influences the observed material response. Four DEM samples with identical initial states were produced: three cylindrical samples bounded by rigid walls and one bounded by a cubical periodic cell. When subjected to triaxial loading, the samples with rigid boundaries were more dilative, stiffer and reached a higher peak stress ratio than the sample enclosed by periodic boundaries. For the rigid-wall samples, dilatancy increased and stiffness decreased with increasing sample size. The periodic sample was effectively homogeneous. The void ratio increased and the contact density decreased close to the rigid walls. This heterogeneity reduced with increasing sample size. The positions of the critical state lines (CSLs) of the overall response in e-log p’ space were sensitive to the sample size, although no difference was observed between their slopes. The critical states of the interior regions of the rigid-wall-bounded samples approached that of the homogeneous periodic sample with increasing sample size. The ultimate strength of the material at the critical state is independent of sample size.

Keywords Discrete element method; Sample size; Rigid boundary; Periodic boundary; Critical state

1. Introduction

The discrete element method (DEM) has been widely used in geotechnical engineering since it was proposed by Cundall and Strack (1979). Most of the published research in geomechanics which uses DEM considers simulations of element tests to study fundamental aspects of soil response (Cui, O’Sullivan, & O’Neill, 2007; Kwok & Bolton, 2010; Yan & Dong, 2011). The computational cost limits the number of particles used in these simulations; around 10,000 particles are commonly used in 3D simulations. For physical laboratory testing, the ratio of sample
size to particle size is usually larger than this, e.g., Head (1994) suggested that the sample thickness should not be less than 10 times the maximum particle diameter in shear box tests. Adhering to these guidelines when running DEM simulations is difficult, particularly when realistic gradings are used, as many small particles must be simulated for every large particle. The presence of these smaller particles significantly increases the number of degrees of freedom in the system and also necessitates the use of a very small timestep to ensure numerical stability. A number of prior studies have considered sample size effects in DEM simulations. Potyondy and Cundall (2004) observed that the bulk properties of bonded materials, e.g., Young’s modulus, are sensitive to the size of the specimen. Kuhn and Bagi (2009) found that compressive strength decreases as specimen size is increased. It has also been found that there is a minimum requirement for the number of particles in order to yield consistent behaviour of the numerical assemblies with different sizes (Collop, McDowell, & Lee, 2004; Plassiard, Belheine, & Donzé, 2009). However, explanations for these phenomena have not been provided in the literature and none of these previous studies have examined the effect of specimen size on the mechanical behaviour of granular materials using a realistic particle size distribution (PSD), which is essential for fair comparison of the numerical simulations and the laboratory tests.

Previous research that has considered boundary effects includes Chan and Ng (1986) who observed relatively high porosities in the vicinity of rigid wall boundaries. Marketos and Bolton (2010) highlighted that porosity, strain and contact force distributions adjacent to the boundaries differ from those within the bulk material. In this paper, we extend these existing research contributions by considering samples with a realistic PSD. The effect of sample size is linked to sample inhomogeneity using detailed particle-scale analyses. The data are interpreted within a critical state soil mechanics (CSSM) framework.

2. DEM sample preparation

The first step in a DEM simulation of an element test is to generate a particle assembly with a specified packing and stress state. Three cylindrical samples enclosed by rigid walls (RW) were created using the PFC3D software (Itasca Consulting Group, 2008) and a fourth sample enclosed
by periodic boundaries (PB) was created using a modified version of the open-source LAMMPS code (Plimpton, 1995). For all these samples, the PSDs were close to the grading curve of Toyoura sand (Yang & Sze, 2011), and the gradings were generated by discretizing the Toyoura grading into several size classes. The particle diameters were assumed to be uniformly distributed within each of these size classes. Particles with a diameter below 0.1156 mm were ignored because their contribution to the overall volume-based PSD is negligible. The simplified Hertz-Mindlin contact model was used. The particle shear modulus ($G$) and Poisson’s ratio ($\nu$) were taken to be 29 GPa and 0.12 respectively following the properties of quartz (Simmons & Brace, 1965). Gravity was not simulated and the rigid walls were frictionless. The four numerical samples are shown in Fig. 1, their PSDs are given in Fig. 2, and key properties of each sample are listed in Table 1. By reference to Fig. 2 and Table 1, it can be seen that the PSDs of all four samples are similar.

Figs. 1 & 2, & Table 1

Considering the rigid-wall samples, the smallest sample, RW-S, had 6783 particles, the medium sample, RW-M, contained 16,073 particles, and the largest cylindrical sample, RW-L, contained 31,392 particles. For these rigid-wall simulations, an initial non-contacting cloud of particles at half of their target sizes was randomly generated. The domain considered was confined by a closed, rigid, cylindrical wall in the lateral direction and two rigid, flat walls in the vertical direction. Large particles were placed within the simulation domain prior to small ones. The particles were then uniformly expanded to their final sizes and the sample was cycled to equilibrium. During this procedure, no wall movement was allowed. A servo-control mechanism was then introduced to adjust both the positions of the flat walls and the radius of the cylindrical wall until an isotropic stress state of 500 kPa was attained. Different coefficients of friction were adopted during the sample preparation stage (0.07 for RW-S, 0.10 for RW-M, and 0.14 for RW-L) to achieve similar void ratios (0.649–0.65) before shearing, as noted in Table 1. For all simulations, the inter-particle friction coefficient was increased to 0.25 prior to shearing. At the onset of shearing, the ratios of sample diameter to the maximum particle diameter were around 7.2, 9.6, and 12 for RW-S, RW-M, and RW-L, respectively. The coordination number ($Z$) and the deviatoric fabric ($\Phi_d$) were used to characterise the samples at the particle scale. The coordination number is
given by $Z = 2N_c / N_p$, where $N_c$ is the number of contacts and $N_p$ is the number of particles.

There is a slight decrease in $Z$ with increasing sample size from 4.64 (RW-S) to 4.37 (RW-L). The deviatoric fabric, $\Phi_d$, is the difference between the maximum and minimum eigenvalues of the fabric tensor of the contact normals as defined by Satake (1982). The maximum $\Phi_d$ value is 0.011, indicating an isotropic packing in all cases.

The periodically-bounded sample, PB, contained 20,164 spherical particles and was generated and sheared using a modified version of the DEM code LAMMPS. The primary modification was to include a stress-control algorithm for periodically-bounded samples. The code was successfully validated using the expressions developed by Thornton (1979) for the peak stress ratios in a face-centred cubic assembly of uniform rigid spheres subjected to plane strain and triaxial conditions. To create the sample for this study, a non-contacting ‘cloud’ of particles was initially generated within a cubical periodic cell using an in-house MATLAB script (The MathWorks Inc., 2011). Starting from the largest, the radii of the particles were successively determined from the upper and lower limits of each size class assuming a uniform distribution in between. When the accumulated particle volume within a size class approximated the target volume allocated to this size class, the algorithm moved to the next size class. Once all particle radii had been determined, the radii were sorted in descending order. Particles were then sequentially placed within the designated domain. During the placement, particles were allowed to intersect the periodic boundaries but were not permitted to overlap each other. Once all particles had been placed within the simulation domain, the sample was initially compressed to a stable stress state of 500 kPa using a coefficient of friction of 0.28. Then the coefficient of friction was set to the final value of 0.25 and the sample was again returned to a stable stress state of 500 kPa. The void ratio after isotropic compression was 0.646. The average ratio of the dimensions of PB to the maximum particle diameter was about 12.5 before shearing. The $\Phi_d$ value for PB was 0.004: lower than the values of all PFC3D samples. The coordination number of PB was 4.37 which was identical to the value for the largest rigid-wall sample, RW-L.
3. Macro-scale behaviour

Fig. 3 illustrates the variation of stress ratio ($q/p'$) with axial strain. The deviatoric stress $q$ is defined as the difference between the major and minor principal stresses while the mean effective stress, $p'$, is the mean value of the three effective principal stresses ($p' = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$). It is clear that the samples behave quite differently from the onset of shear deformation. All the rigid-wall samples are stiffer than sample PB; however, their stiffness reduces with increasing sample size. The smallest rigid-wall sample, RW-S, mobilized the highest peak stress ratio. Jefferies, Been, and Hachey (1990) observed in laboratory tests that large specimens showed a brittle strain softening behaviour post peak, while their small specimen was more ductile. They attributed it to the formation of multiple shear bands in large specimens. However, shear band formation was not observed in the DEM simulations. This may explain why the difference in the post-peak responses is less marked than in the laboratory tests.

In the framework of CSSM, soils which have been sheared to a large strain level will deform continuously without a change of volume and stress state. This state is defined as the critical state (Roscoe, Schofield, & Wroth, 1958). In the DEM simulations, all the samples reached an almost identical stress state at large strain levels (Fig. 3), suggesting that the ultimate strength at the critical state is the unique property of materials and is independent of the sample size and boundary conditions. Though they did not shear their specimens to the critical state, Jefferies et al. (1990) also expected the convergence of shear strengths of differently-sized specimens at large strain levels. Considering the volumetric strain response which is illustrated in Fig. 4, the rigid-wall samples firstly contracted and then dilated until the critical state was attained. This transition from a contractive to a dilative response occurred at a much larger strain level in RW-L than in the smaller rigid-wall samples. The periodically-bounded sample, PB, behaves contractively throughout shearing. The largest rigid-wall sample, RW-L, is significantly less dilative than the smallest PFC sample, RW-S. This sample-size effect is in agreement with the observation of Jefferies et al. (1990). The void ratios at the end of the simulations are 0.676, 0.663, 0.656, and 0.630 for RW-S, RW-M, RW-L, and PB, respectively. Overall, the rigid-wall samples behave as if they are “dry”, or denser than the critical state, while the periodically-bounded sample
PB exhibits a “wet” condition, indicative of a sample whose initial state is above the critical state corresponding to the same $p'$. 

Figs. 3 & 4

4. Evaluation of homogeneity of samples at the initial state

The homogeneity of the samples at the initial state was evaluated to explain the differences in specimen response. To quantify the homogeneity in the vertical direction, the cylindrical rigid-wall samples were divided into eight horizontal slices or layers (Fig. 5(b)). The lateral homogeneity of the rigid-wall samples was studied by looking at 4 cylindrical zones (rings) extending from the bottom rigid wall boundary to the top boundary (Fig. 5(c)). The sample PB was studied by looking at the corresponding eight isochoric slices whose thicknesses are larger than twice the maximum particle diameter. Both horizontal and vertical directions were considered (Fig. 5(d)).

The initial analysis considered the void ratio. As illustrated in Fig. 5(a), the solid volume in each slice was accurately considered by introducing the analytical expression for the spherical crown volume (Eq. (1)) and the analytical expression for the volume of intersection between a sphere and a cylinder based on elliptical integrals (Lamarche & Leroy, 1990).

$$V_{\text{inter}} = \pi h^2 \left( r - \frac{h}{3} \right), \quad (1)$$

where $h$ and $r$ are defined in Fig. 5(a). The solid volume within a given zone was the summation of the volume of fully-enclosed particles and that of intersected boundary particles whose fractions outside the zone were subtracted. As shown in Fig. 5(b), (c) and (d), the volume of particles intersected by the lower/inner bound of the current zone was added to the solid volume of the previous zone, while the volume of particles intersected by the upper/outer bound of the current zone was added to the solid volume of the next zone. The solid volumes that lay outside the rigid boundaries according to these calculations were ignored as they were only the contact overlap between particles and walls and contributed little to the overall solid volume. However,
the solid volume beyond the bottom/top periodic boundary was added into the zone containing the top/bottom boundary according to their actual mechanical contributions. The solid volume outside the lateral periodic boundaries was fully considered as this part would act effectively on the opposite side.

Fig. 5

The distributions of void ratio normalized by the overall average void ratio for each sample are shown in Fig. 6 for the rigid-wall samples, while Fig. 7 illustrates the distribution of normalized void ratios in sample PB. Referring to Fig. 6, it is clear that the void ratios in the boundary regions of the rigid-wall samples are higher than the overall average value while the void ratios of the interior regions are lower than the average value in both the vertical and radial directions. The difference between the boundary void ratio and interior void ratio is more obvious in the radial direction than in the axial direction and decreases when the sample becomes larger. In contrast, Fig. 7 shows an almost uniform distribution of void ratio for the PB sample. The calculated unbiased sample variances of void ratio have been used to quantify the degree of homogeneity by Jiang, Konrad, and Leroueil (2003) and are also adopted here. These variances of void ratio are given by:

$$S^2 = \frac{1}{m-1} \sum_{i=1}^{m} (e_i - e_{\text{overall}})^2,$$  \hspace{1cm} (2)$$

where $m$ is the total number of slices, $e_i$ is the void ratio within zone $i$ and $e_{\text{overall}}$ is the overall void ratio. The variances of void ratio of the numerical assemblies used in this study are given in Table 2. It is clear that the periodically-bounded sample, PB, has the lowest variances and they are very small in all three Cartesian directions. Moreover, the rigid-wall samples have larger variances in the radial direction than in the vertical direction and the variances decrease with increasing sample size. This may be because the outermost zone in the radial direction contained the entire cylindrical boundary and a fraction of top and bottom boundaries as well, while the outermost zones in the vertical direction contain only the top/bottom rigid wall and a small portion of the cylindrical boundary. With an increase in sample size, there is more space for the placement of
particles at the boundaries.

**Figs. 6 & 7, Table 2**

At the particle scale, the packing inhomogeneity can be calculated by considering the contact density, i.e., the number of contacts per unit volume. Figs. 8 and 9 present the distribution of initial contact density within the rigid-wall samples and the periodically-bounded sample, respectively. For each sample, the contact densities which are presented were normalized by the overall average contact density within the sample. Although the samples are quite uniform in the interior regions, there is a considerable reduction in the contact density in the boundary regions of samples generated using rigid boundaries (Fig. 8), while the contacts are uniformly distributed within the periodically-bounded sample (Fig. 9). The variances of contact density are given in Table 3. As was the case for the void ratio data, the variances of contact density of the periodically-bounded sample are very small in all three directions, while those of the rigid-wall samples are much larger. The variation of contact density in the rigid-wall samples is more obvious in the radial direction than in the vertical direction. Increasing the sample size reduces the heterogeneity of the sample, as was the case for the void ratio.

**Figs. 8 & 9, Table 3**

The volumetric PSDs of different parts of the rigid-wall samples were determined and their main characteristics are summarized in Table 4. In this table, slices 2–7 in the vertical direction are grouped to form the “middle” region, material in rings 1–3 in the radial direction (grouped together) are considered to be the “inner” region, horizontal layers 1 and 8 are the “boundary” regions and ring 4 is the “outer” region. There is indeed a higher proportion of small particles near the boundaries than in the interior regions. However, this difference is not significant and becomes almost unnoticeable in the larger samples, RW-M, and RW-L.

**Table 4**
5. Critical state behaviour

Many research studies have demonstrated that the critical state line (CSL) is linear in $e^{-\left(p'/p'_a\right)\alpha}$ space and the position of this line is a unique property of a given material (Roscoe et al., 1958). The critical states of the entire samples and their interior parts (Fig. 5(c) zones 1, 2, and 3) were analysed separately. Fig. 10 shows the critical state of the DEM samples plotted in the $e$ against $\left(p'/p'_a\right)\alpha$ space, where $\alpha$ is a material parameter taken here to be 0.7 (the usual value for Toyoura sand (Li & Wang, 1998)) and $p_a$ is atmospheric pressure (taken here to be 101.3 kPa). In Fig. 10, hollow symbols show the initial states, while solid symbols represent the critical states. The CSLs are the best-fit results of the cases discussed in Section 3 and some other supplemental simulations. The CSL of RW-L is absent as only one simulation was completed due to the high computational cost.

As shown in Fig. 10, all the CSLs are parallel to each other with almost identical slopes of around 0.001. The CSL of the RW-S sample lies above the CSL of the RW-M sample and the CSL of the PB samples is located below all the rigid-wall samples, i.e., the CSL moves downwards as the specimen size increases for the rigid-wall samples. The intercepts of the CSLs decrease with increasing specimen size, while the slopes seem to be less sensitive to the specimen size. The state parameter $\psi$ is defined as the difference between the current void ratio and the void ratio at the critical state corresponding to the same mean effective stress (Been & Jefferies, 1985). Specimens with a higher $\psi$ are looser and behave more contractively than specimens with a lower $\psi$. The state parameters for the RW-S and RW-M samples are $-0.027$ and $-0.014$, respectively. Therefore, when sheared under triaxial loading conditions, the RW-M should be more contractive than the RW-S.

These observations seem to violate the principles of classical CSSM which propose that the CSL is a unique characteristic of a material. Considering the inhomogeneity induced by the rigid walls, the stresses and strains measured at the boundary may not accurately reflect the real material response. Hence, we consider the interior parts of all the samples together to interpret the
critical state behaviour. The average macro stresses of the middle/inner parts of the rigid-wall samples were calculated from average stresses of particles centred within these zones weighted by their volumes (O’Sullivan, 2011).

\[
\bar{\sigma}_{ij} = \frac{1}{N_p} \sum_{p=1}^{N_p} \bar{\sigma}_{ij}^p \cdot V^p,
\]

(3)

where \(\bar{\sigma}_{ij}\) is the average stress tensor within the region of interest, i.e., the interior parts of the rigid-wall samples, \(N_p\) is the total number of particles and \(\bar{\sigma}_{ij}^p\) is a representative stress tensor for a single particle of volume \(V^p\). The critical states of the interior parts of the rigid-wall samples are also shown in Fig. 10. It is interesting to see that they all approach the CSL of the periodically-bounded samples. This suggests that the critical state behaviour is unique and independent of the specimen size given that the stresses and strains are correctly interpreted by eliminating the boundary effect.

Fig. 11 shows the stress state at the critical state in terms of \(q\) and \(p'\). All \((q, p')\) points at the critical state can be represented by a single straight line irrespective of the specimen size and boundary conditions. The slope \((M)\) of this straight line is about 0.69. This corresponds to an angle of shearing resistance of 18° at the critical state, calculated from

\[
\phi_{\infty} = \sin^{-1} \left( \frac{3M}{6 + M} \right).
\]

(4)

The angle of shearing resistance at the critical state represents the ultimate resistance of the material to shearing and is found here to be independent of the specimen size.

The values of \(Z\) and \(\Phi_d\) at the critical state for all samples are given in Table 5. The value of \(Z\) decreases with decreasing size for the rigid-wall samples. This concurs with the observation of void ratios above, showing that the sample PB is the densest at the end of the simulation and the void ratio at the critical state decreases with increasing the sample size. It is interesting to note that
while the $\Phi_d$ value of the LAMMPS sample remains the smallest, the $\Phi_d$ values of the rigid-wall samples are almost identical to each other and the difference in the $\Phi_d$ values between the rigid-wall samples and the periodically-bounded sample is smaller than at the initial state.

Table 5

6. Conclusions

In a DEM study of behaviour in triaxial compression, three differently-sized samples bounded by rigid boundaries were created and compared with a sample enclosed by periodic boundaries. All the samples had an almost identical initial void ratio and stress state before being subjected to triaxial shearing. The rigid-wall samples were stiffer than the periodically-bounded sample and behaved more dilatively. Here we argue that these differences are a consequence of the different degrees of homogeneity in the samples at the initial state. While periodic boundaries yield a homogeneous sample, the adoption of rigid boundaries causes an increase of void ratio and a reduction of contact density in the vicinity of the rigid boundaries. This heterogeneity seemed to be more obvious in the radial direction than in the vertical direction and to decrease with increasing sample size. We propose here that the high void ratio and low contact density at the boundary areas relative to the interior regions may make the stress-strain conventionally measured at the boundaries not representative of the real material responses.

The sample size effect can be explained in the framework of CSSM. It is observed that the location of the CSL depends on the boundary conditions and the sample size. The CSLs of samples bounded by rigid boundaries locate above the CSL of the periodically-bounded sample, while the slope of the CSL in the $e-(p'/p'_a)\alpha$ space seemed to be dependent on neither the sample size nor the boundary conditions. The stress-strain responses of the samples differ due to the different relative positions of initial states to the critical states. Furthermore, the critical states of the interior part of rigid-wall samples approach the CSL of the homogeneous periodically-bounded sample with an increase of sample size, indicating that the interior parts of rigid-wall-bounded samples are the most representative of the real material behaviour. The ultimate strength of the material is independent of the specimen size as well as the boundary
conditions.

The findings of this study indicate:

(1) The kinematic and geometrical constraint imposed by the rigid wall boundaries results in an inhomogeneity in the packing density (i.e., void ratio and contact density) of the samples. The soil response in this region is significantly influenced by this constraint and is not representative of the overall material behaviour. In smaller samples, the volume of material influenced by this kinematic constraint is sufficiently large, relative to the sample volume, that this constraint influences the observed overall stress-deformation response. Analysis of the particle size distribution did not reveal sufficient variation to contribute to the differences in response.

(2) The application of periodic boundaries may be beneficial as it yields a more homogeneous sample and deformation field than rigid boundaries and thus is more likely to capture the real material responses.

(3) When rigid boundaries are used, the sample size should be large enough to reduce the influence of the kinematic boundary constraint which has a major impact on the overall mechanical behaviour of granular materials. Otherwise, the DEM results may not reflect the real material behaviours correctly, e.g., the CSL.

(4) It may also be beneficial, where using rigid wall boundaries, to generate initially large blocks and then numerically carve the cylindrical samples from these large blocks to obtain homogeneous samples. This approach was adopted by Cheung (2010).

(5) In DEM simulations with rigid wall boundaries, the response of an inner region or sub-volume should be compared with the overall material response to demonstrate that the overall response is representative of the material.

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code development, was provided as part of grant EP/I006761/1 from the Engineering and Physical Sciences Research Council.

References


**Figures**

Fig. 1. Schematic diagrams of four numerical samples.
Fig. 2. Realistic particle size distributions of four numerical samples.

Fig. 3. Variations of stress ratio with axial strain for four numerical samples.
Fig. 4. Volumetric strain response for four numerical samples.
Fig. 5. The homogeneity of the samples at the initial state: (a) solid volume within each zones, (b) cylindrical rigid-wall samples at vertical direction, (c) cylindrical zones (rings) extending from bottom rigid wall boundary to top boundary, and (d) sample PB at horizontal and vertical directions.
Fig. 6. Distributions of initial void ratio of rigid-wall samples in which the shading illustrates data values normalized by the mean void ratio ($e_0 = 0.649$) for each sample and the actual void ratio values in each region are given on the right side of each plot.

Fig. 7. Distributions of initial void ratio of the periodically-bounded sample in which the shading indicates void ratios normalized by the mean for the entire sample ($e_0 = 0.646$) and the actual void ratios in each region are given on the right side of each plot.
Fig. 8. Distributions of initial contact density of rigid-wall samples in which the shading illustrates data values normalized by the mean contact density for each sample and the actual contact densities in each region are given on the right side of each plot. (The mean contact densities for RW-L, RW-M, and RW-S are 331, 346, and 361 mm⁻³, respectively.)

Fig. 9. Distributions of initial contact density of periodically-bounded sample in which the shading indicates contact densities normalized by the mean contact density for the entire sample and the actual contact densities in each region are given on the right side of each plot. (The mean contact density for PB sample is 301 mm⁻³.)
Fig. 10. The critical state of DEM samples plotted in the $e$ against $(p'/p_a)^{0.3}$ space.

Fig. 11. The stress state at the critical state in terms of $q$ and $p'$. 
### Tables

**Table 1** Initial characteristics of the prepared virtual samples and a real Toyoura sand for comparison

<table>
<thead>
<tr>
<th>Sample</th>
<th>Number of particles</th>
<th>$D_{50}$ (mm)</th>
<th>$C_u$</th>
<th>$C_c$</th>
<th>$e_0$</th>
<th>Z</th>
<th>$\Phi_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RW-S</td>
<td>6783</td>
<td>0.216</td>
<td>1.490</td>
<td>0.943</td>
<td>0.649</td>
<td>4.64</td>
<td>0.011</td>
</tr>
<tr>
<td>RW-M</td>
<td>16,073</td>
<td>0.215</td>
<td>1.488</td>
<td>0.951</td>
<td>0.649</td>
<td>4.51</td>
<td>0.0091</td>
</tr>
<tr>
<td>RW-L</td>
<td>31,392</td>
<td>0.214</td>
<td>1.478</td>
<td>0.953</td>
<td>0.650</td>
<td>4.37</td>
<td>0.0081</td>
</tr>
<tr>
<td>PB</td>
<td>20,164</td>
<td>0.218</td>
<td>1.386</td>
<td>0.983</td>
<td>0.646</td>
<td>4.37</td>
<td>0.004</td>
</tr>
<tr>
<td>Toyoura sand</td>
<td>–</td>
<td>0.216</td>
<td>1.392</td>
<td>0.961</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

$C_u$: coefficient of uniformity, $C_c$: coefficient of curvature, $e_0$: initial void ratio, Z: coordination number, $\Phi_d$: deviatoric fabric

**Table 2** Unbiased sample variance of initial void ratio

<table>
<thead>
<tr>
<th></th>
<th>RW-S</th>
<th>RW-M</th>
<th>RW-L</th>
<th>PB</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Vertical</td>
<td>Radial</td>
<td>Vertical</td>
<td>Radial</td>
</tr>
<tr>
<td>$S^2$</td>
<td>0.0007</td>
<td>0.0054</td>
<td>0.0004</td>
<td>0.0031</td>
</tr>
</tbody>
</table>

**Table 3** Unbiased sample variance of initial contact density

<table>
<thead>
<tr>
<th></th>
<th>RW-S</th>
<th>RW-M</th>
<th>RW-L</th>
<th>PB</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Vertical</td>
<td>Radial</td>
<td>Vertical</td>
<td>Radial</td>
</tr>
<tr>
<td>$S^2$ (mm$^{-6}$)</td>
<td>706.45</td>
<td>4674.86</td>
<td>553.57</td>
<td>2524.18</td>
</tr>
</tbody>
</table>
Table 4 Characteristics of PSDs in different parts of the rigid-wall samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>$D_{50}$ (mm)</th>
<th>$C_u$</th>
<th>$C_c$</th>
<th>$D_{max}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RW-S-middle</td>
<td>0.218</td>
<td>1.5</td>
<td>0.936</td>
<td>0.4117</td>
</tr>
<tr>
<td>RW-S-bound</td>
<td>0.209</td>
<td>1.461</td>
<td>0.966</td>
<td>0.3838</td>
</tr>
<tr>
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<td>1.50</td>
<td>0.942</td>
<td>0.4117</td>
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<tr>
<td>RW-S-outer</td>
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<td>1.482</td>
<td>0.944</td>
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<tr>
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<tr>
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<td>1.479</td>
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<tr>
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<td>1.485</td>
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Table 5 Micro characteristics of samples at the critical state

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<th>RW-L</th>
<th>PB</th>
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<tr>
<td>$Z$</td>
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<td>4.18</td>
<td>4.22</td>
<td>4.39</td>
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<td>0.090</td>
<td>0.089</td>
<td>0.086</td>
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