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A new suggestion for determining 2D porosities in DEM studies

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Abstract. In discrete element modeling, 2D software has been widely used in order to gain further insights into the fundamental mechanisms with less computational time. The porosities used in 2D DEM studies should be determined with appropriate approaches based on 3D laboratory porosities. This paper summarizes the main approaches for converting porosities from 3D to 2D for DEM studies and theoretical evaluations show that none of the current approaches can be widely used in dealing with soil mechanical problems. Therefore, a parabolic equation and a criterion have been suggested for the determination of 2D porosities in this paper. Moreover, a case study has been used to validate that the 2D porosity obtained from the above suggestion to be rational with both the realistic contact force distribution in the specimen and the good agreement of the DEM simulation results of direct shear tests with the corresponding experimental data. Therefore, the parabolic equation and the criterion are suggested for the determination of 2D porosities in a wide range of polydisperse particle systems, especially in dealing with soil mechanical problems.

Keywords: discrete element method (DEM); 2D porosity; criterion; soil mechanics; Particle Flow Code (PFC)

1. Introduction

The discrete element method (DEM) (Cundall and Strack 1979), which has particular advantages of capturing detailed insights into the kinematic behaviour of discontinuous media, has been widely used in investigating the mesoscopic behaviour of granular materials (Nicot *et al*. 2007, 2011, Li *et al*. 2013). Hence, the DEM has been regarded as a powerful supplement to conventional laboratory tests and numerical simulations based on finite element method (FEM) (Meier *et al*. 2008, Rahmati *et al*. 2014).

It is well known that DEM simulation results are highly determined by the selected models and the corresponding input parameters, e.g. contact stiffness and friction coefficient of the particles and walls, modulus, damping, Poisson's ratio, etc. Many studies have focused on the influences of those input parameters on the material behaviour (Härtl and Ooi 2008, Abbireddy and Clayton 2010, Mohamed and Gutierrez 2010). The effects of all the above parameters, however, are all based on certain particle packing with defined porosities. The porosities used in 3D DEM studies

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can be determined from laboratory porosities directly, whilst the porosities used in 2D DEM investigations should be determined with appropriate approaches based on laboratory porosities since an area-based 2D porosity is entirely different from a volume-based 3D porosity. Moreover, compared with 3D software, 2D software has the advantage of giving insights into key phenomena and mechanisms with less computational time, which leads to a wide usage of 2D software in investigating geomechanical problems (Wang and Leung 2008, Bhandari and Han 2010, Jiang *et al*. 2011, Jia *et al*. 2013, Zhang *et al*. 2013, Ai *et al*. 2014). Therefore, selecting an appropriate approach to determine the 2D porosity in DEM studies is the foremost step for all 2D DEM simulations and further analyses. After fixing the 2D porosity, the calibrations of the models and the input parameters can be proceeded in further DEM studies.

The approaches for linking 2D and 3D porosities have been suggested in many studies (Hoomans *et al*. 1996, Ouyang and Li 1999, Van Wachem *et al*. 2001, Bezuijen and van den Berg 2002, Giese 2002, Hainbüchner *et al*. 2002, Helland *et al*. 2005, Zhang 2007). However, the relations between 2D and 3D porosities up to now have not been investigated conclusively, which still causes empirical selections of 2D porosities for DEM studies (Wang and Leung 2008, Han *et al*. 2012, Bhandari *et al*. 2014). Moreover, due to varying particle size distributions of soil in practice, it might be impossible just to use a specific equation to link 2D and 3D porosities especially for arbitrary assemblies with polydisperse particle systems.

In this paper, different approaches for converting porosities from 3D to 2D have been summarized and theoretically evaluated. A parabolic equation and a criterion have been suggested for determining 2D porosities in DEM studies. Moreover, further DEM simulations have been conducted to validate that the 2D porosity obtained from the above suggestion to be rational. All the DEM simulations in this study have been conducted using PFC^{2D}.

2. Current approaches

Currently, there are six approaches commonly used to link 2D and 3D porosities for DEM studies. All those methods are summarized and evaluated as follows.

2.1 Individual illustration of each approach

(1) The Densest State Method

Assuming particles with identical diameters in both 2D and 3D, Hoomans *et al*. (1996) derived Eq. (1) by matching a 2D hexagonal lattice structure and a 3D face centered cubic (FCC) structure. Since the hexagonal lattice structure and the FCC structure represent the densest 2D and 3D packing in mono-sized systems, the following equation is named as the Densest State Method in this study

$$n_{2D} = 1 - [\frac{\sqrt{\pi\sqrt{3}}}{2} \cdot (1 - n_{3D})]^{2/3} \tag{1}$$

where n_{2D} and n_{3D} are the porosities in 2D and 3D, respectively.

The Densest State Method has also been used by Lin *et al*. (2013) to simulate sandy soil reinforced with H-V inclusions in plane strain tests.

Van Wachem *et al*. (2001) modified the Densest State Method by introducing an empirical parameter containing the maximum experimental solids packing in practice.

$$n_{2D} = 1 - [\frac{\sqrt{\pi\sqrt{3}}}{2\nu} \cdot (1 - n_{3D})]^{2/3} \tag{2}$$

where $\nu = \frac{n_{lab,\min}}{n_{3D,\min}}$; $n_{lab,\min}$ and $n_{3D,\min}$ are the minimum 3D porosities in laboratory tests and theoretical calculations, respectively.

(2) The Loosest State Method

With a similar derivation process of the Densest State Method, the Loosest State Method is obtained by matching a 2D square packing and a 3D simple cubic structure which represent the loosest 2D and 3D packing in mono-sized systems, as shown in Eq. (3). Helland *et al*. (2005) used the identical equation in a numerical study of cluster and particle rebound effects in a circulating fluidized bed, but they utilized a pseudo-3D concept in which they assumed that the depth of the fluidized bed was equal to the particle diameter.

$$n_{2D} = \frac{3}{2} n_{3D} - \frac{1}{2} \tag{3}$$

(3) Interval Mapping Method

Ouyang and Li (1999) proposed the Interval Mapping Method, as shown in Eq. (4). They verified their method by comparing a 2D hexagonal lattice structure with a 3D hexagonal packed structure. Both structures were based on mono-sized systems.

$$n_{2D} = 1 - [\frac{\sqrt{\pi\sqrt{3}}}{\sqrt{2}} \cdot (1 - n_{3D})]^{2/3} \tag{4}$$

(4) Combination Method

Zhang (2007) combined the Densest State Method and the Interval Mapping Method by introducing the relative density D_r, which represents different density states in soil mechanics. The Combination Method is illustrated as follows

$$n_{2D} = 1 - (\frac{1 - n_{lab}}{\xi})^{2/3} \tag{5}$$

where $\xi = \frac{\sqrt{2}}{\sqrt{\pi\sqrt{3}}} + D_r \cdot (\frac{2}{\sqrt{\pi\sqrt{3}}} - \frac{\sqrt{2}}{\sqrt{\pi\sqrt{3}}})$; $D_r = \frac{e_{\max} - e}{e_{\max} - e_{\min}}$; $e_{\max}$, $e_{\min}$ and e are the maximum, the minimum and the test void ratios in laboratory tests, respectively.

It should be noted that when $D_r = 0$, the Combination Method is the same as the Interval Mapping Method; when $D_r = 1$, the Combination Method is identical to the Densest State Method.

(5) Linear Interpolation Method (LIM)

The definition of density in soil mechanics can also be used to convert porosities from 3D to

2D. The Linear Interpolation Method is based on the assumption that the degree of densities in both 2D and laboratory tests (3D) are identical.

The degree of densities depending on the maximum, the minimum and the test porosities in both 2D and laboratory tests can be expressed by

$$D = \frac{n_{2D,\max} - n_{2D}}{n_{2D,\max} - n_{2D,\min}} = \frac{n_{lab,\max} - n_{lab}}{n_{lab,\max} - n_{lab,\min}} \tag{6}$$

where $n_{2D,max}$, $n_{2D,min}$ and n_{2D} are the maximum, the minimum and the test porosities in 2D ($n_{2D,max} \approx 0.2146$ and $n_{2D,min} \approx 0.0931$), $n_{lab,max}$, $n_{lab,min}$ and n_{lab} are the maximum, the minimum and the test porosities in laboratory tests.

Transforming Eq. (6), the test 2D porosity can be computed with the following equation

$$n_{2D} = n_{2D,\max} - D \cdot (n_{2D,\max} - n_{2D,\min}) \tag{7}$$

where $D = \frac{n_{lab,\max} - n_{lab}}{n_{lab,\max} - n_{lab,\min}}$.

Using the Linear Interpolation Method, Giese (2002) and Hainbüchner *et al*. (2002) conducted numerical simulations of vibroflotation compactions and shallow foundation stabilities, respectively.

(6) Quasi 3D Porosity Method

The Quasi 3D Porosity Method was based on the assumption that the diameter and thickness of the “2D discs” were equal to the diameter of the sphere (Bezuijen and van den Berg 2002). After comparing the volume equations of the disc and the sphere, a quasi 3D porosity equation was proposed to compute the maximum and minimum quasi 3D porosities ($n'_{3D,max}$ and $n'_{3D,min}$) with the following equations

$$n'_{3D,\max} = \frac{1}{3} + \frac{2}{3} n_{2D,\max} \tag{8}$$

$$n'_{3D,\min} = \frac{1}{3} + \frac{2}{3} n_{2D,\min} \tag{9}$$

Subsequently, the Linear Interpolation Method was used to calculate the quasi 3D porosity n'_{3D} as follows

$$n'_{3D} = n'_{3D,\max} - \frac{n_{lab,\max} - n_{lab}}{n_{lab,\max} - n_{lab,\min}} \cdot (n'_{3D,\max} - n'_{3D,\min}) \tag{10}$$

Finally, the 2D porosity is obtained with the following equation

$$n_{2D} = \frac{3}{2} n'_{3D} - \frac{1}{2} \tag{11}$$

The computing process of this method can be regarded as the combination of the Loosest State Method and the Linear Interpolation Method.

2.2 Theoretical evaluation of the above approaches

Fig. 1 shows the relations between 2D and laboratory porosities based on different approaches, in which the maximum and the minimum porosities of sand in laboratory tests are 0.4571 and 0.3253, respectively. From Fig. 1 we can see, the 2D porosities obtained based on the Combination Method decrease with increasing laboratory porosities, which is against the general relation between 2D and laboratory porosities. The negative values of 2D porosities based on the Loosest State Method and the Interval Mapping Method demonstrate that both methods cannot be used in dealing with soil mechanical problems. According to the definition of the Densest State Method, this method was proposed based on an extreme packing with mono-sized systems and thus it cannot be used in a wide range of polydisperse particle systems. The Quasi 3D Porosity Method is only applicable to the case that the diameter and thickness of the "2D discs" are equal to the diameter of the sphere. The Linear Interpolation Method illustrated above is highly dependent on the maximum and the minimum porosities in laboratory, as shown in Fig. 2 ($LIM_{2D\text{-}Lab}$). Theoretically, however, the Linear Interpolation Method should be based on matching the 2D square packing and the 2D hexagonal lattice structure with the 3D simple cubic structure and the 3D face centered cubic structure, respectively, as shown in Fig. 2 ($LIM_{2D\text{-}3D}$). The $LIM_{2D\text{-}3D}$ is independent on the maximum and the minimum porosities in laboratory tests. Corresponding to a laboratory porosity of $n_{Lab} = 0.3434$ (dense packing with a relative density of $D_r = 0.89$), the 2D porosity obtained from the $LIM_{2D\text{-}3D}$ is 0.14 and the 2D porosity calculated based on the $LIM_{2D\text{-}Lab}$ is 0.11. The differences of the 2D porosities based on the $LIM_{2D\text{-}3D}$ and the $LIM_{2D\text{-}Lab}$ are compared in Fig. 2. Moreover, due to the varying particle size distributions of soil in practice, it might be impossible just to use a specific equation to link 2D and 3D porosities for polydisperse particle systems.

Therefore, it can be concluded that none of the above approaches can meet the requirements of linking 2D and 3D porosities in a wide range of polydisperse particle systems, especially in

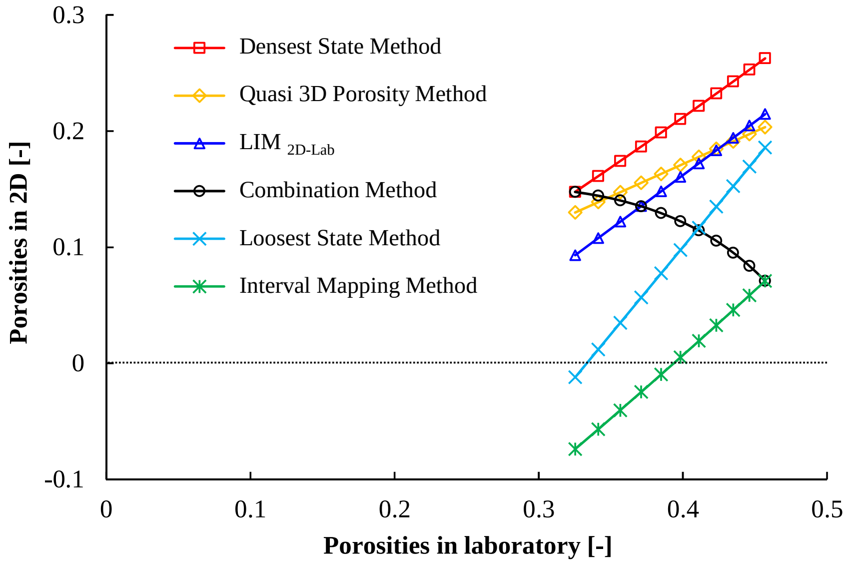


Fig. 1 Relations between 2D and laboratory porosities based on different methods

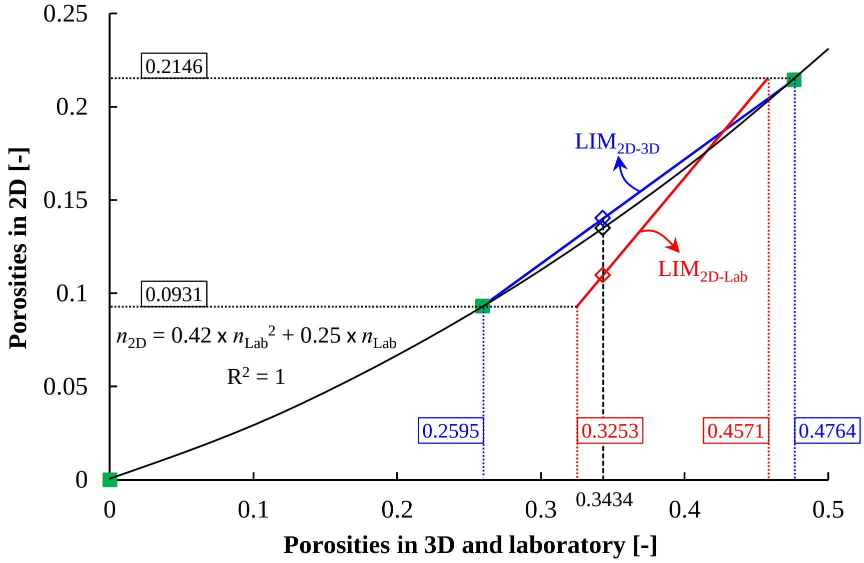


Fig. 2 Relations between 2D and laboratory porosities based on the LIM and the new method

dealing with soil mechanical problems. It is necessary to suggest a reasonable way to link 2D and 3D porosities especially for arbitrary assemblies with various polydisperse particle systems.

3. Illustration of the parabolic equation and the criterion

In this paper, a parabolic equation as well as a criterion have been suggested for determining 2D porosities in DEM studies. Although the $LIM_{2D\text{-}3D}$ is also based on a mono-sized system, the two endpoints of this line segment could still be used as a rough guideline for developing the parabolic equation. Moreover, when the porosity in 3D (or in laboratory) is 0 in a polydisperse particle system, the corresponding 2D porosity should also be 0. Therefore, the initial parabolic equation is obtained based on the above three points, as shown in Fig. 2. It should be noted that the parabolic equation is independent on the maximum and the minimum porosities in laboratory and it is only an initial guideline for converting porosities from 3D to 2D. The parabolic equation is shown as follows

$$n_{2D} = 0.42 \times n_{Lab}^{\ 2} + 0.25 \times n_{Lab} \tag{12}$$

where: n_{2D} is the initial 2D porosity and n_{Lab} is the laboratory porosity.

The final 2D porosity, which can be used for further DEM simulations, is suggested to be determined according to the flow chart in Fig. 3. First of all, preliminary DEM simulations using the initial 2D porosity obtained from Eq. (12) were conducted to record the contact force distribution in the specimen. In this study, the initial 2D porosity was $n_{2D} = 0.14$, which corresponded to the 3D porosity in laboratory tests of $n_{Lab} = 0.3434$. The micro input parameters used in this study are listed in Table 1. It should be noted that the thicknesses of the soil particles along the plane of paper were 8 mm so that the calibration results could be used in further investigations with one geogrid tensile member (Wang *et al*. 2014). Since the computation time in DEM simulations is highly depending on the particle numbers, the particle sizes in laboratory tests were modified and increased with an up-scaling factor of 10, as shown in Fig. 4. The technique of "up-scaling" has been successfully used in previous studies (Wang and Leung 2008, Lin *et al*. 2013, Tran *et al*. 2013, Wang *et al*. 2014). The corresponding number of the soil particles was 2591 ($n_{2D} = 0.14$). The linear contact stiffness model (Itasca 2008) was used to illustrate the contact behaviour of two contacting entities (particle-to-particle or particle-to-wall). The specimens were prepared with a multilayer compaction method (four horizontal layers in this study). For each layer, the standard of the equilibrium state was that the maximum contact force ratio was smaller than 0.001. In order to prepare a dense specimen, a very small friction coefficient of $f_0 = 0.05$ was set to the particles according to the suggestion by Härtl and Ooi (2008). After the last layer reaching the equilibrium state, the friction coefficient of the particles was then increased to a large value ($f_p = 3$ in this study) so as to compensate the lack of angularity for circular particles. Large friction coefficients of particles have also been used in previous studies (Lin *et al*. 2013, Zhang *et al*. 2013, Wang *et al*. 2014) for circular particles in DEM studies. The friction

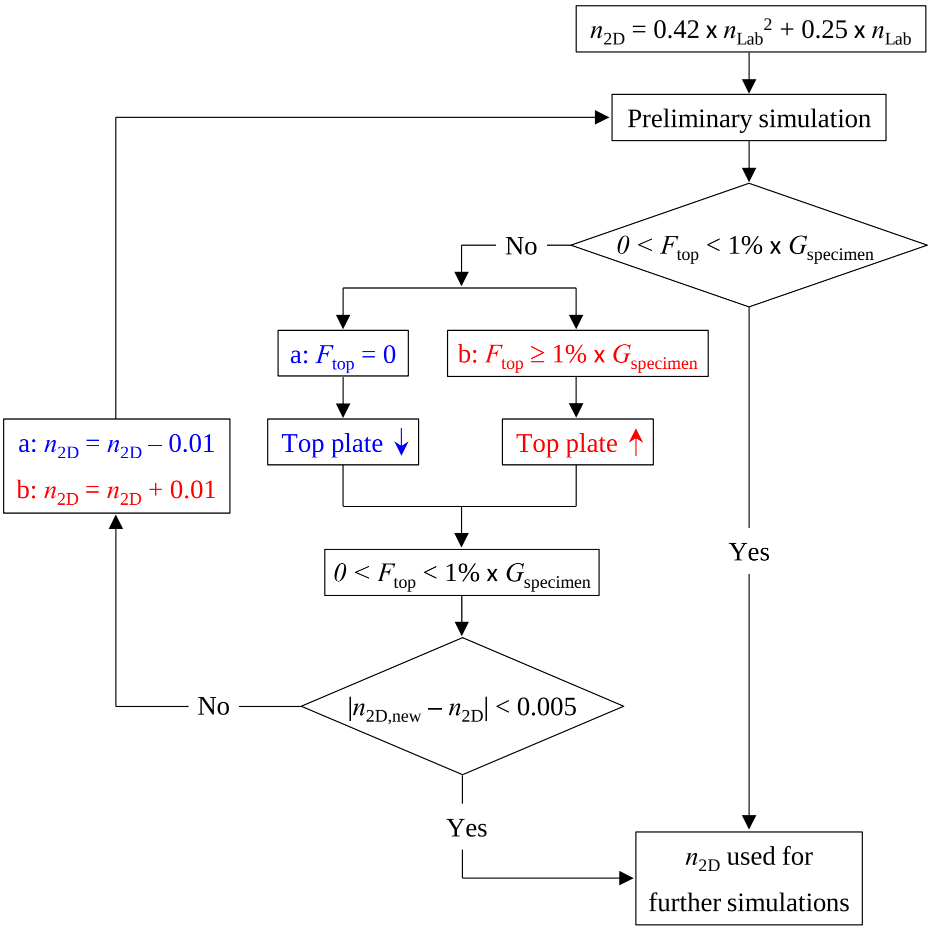


Fig. 3 Flow chart of the criterion for the determination of the final 2D porosity

Table 1 Parameters used in DEM simulations

Width of the specimen W [m]	0.305
Height of the specimen H [m]	0.124
Density of the solids ρ_s [kg/m^3]	2650
Water content w [%]	0
Particle diameters d [mm]	Gradation as in Fig. 4
Normal contact stiffness of the walls $k_{n,w}$ [N/m]	1×10^7
Shear contact stiffness of the walls $k_{s,w}$ [N/m]	1×10^7
Normal contact stiffness of the particles $k_{n,p}$ [N/m]*	4×10^5
Shear contact stiffness of the particles $k_{s,p}$ [N/m]*	4×10^5
Friction coefficient of the particles for specimen preparation f_0 [-]	0.05
Friction coefficient of the particles after specimen preparation f_p [-]	3
Friction coefficient between the particles and the walls f_w [-]	1.5

*The normal and shear contact stiffnesses of the particles were chosen according to similar DEM simulations (Wang and Leung 2008, Jiang *et al*. 2011, Han *et al*. 2012, Lin *et al*. 2013, Zhang *et al*. 2013) and adjusted according to the calibration of the numerical direct shear test results with the corresponding experimental data (Wang *et al*. 2014)

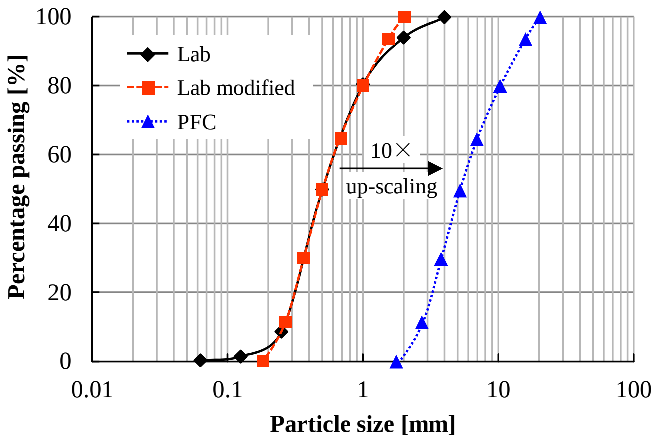


Fig. 4 Particle size distributions in laboratory tests and in DEM simulations

coefficient between the particles and the walls f_w was kept constant during the whole process.

After the prepared specimen reaching the equilibrium state, the top boundary was fixed just to keep the target porosity of $n_{2D} = 0.14$ constant. The vertical force on the top plate of the specimen F_{top} was measured. If F_{top} was greater than 0 but less than 1% of the specimen's weight, it represented that the specimen area was full of particles with the target porosity and meanwhile the contact force distribution in the specimen was regarded to be rational according to the realistic contact force distribution under the gravitational load. Hence, the initial porosity could be used for further simulations. If not, the top plate moved downwards or upwards until F_{top} was greater than 0 but less than 1% of the specimen's weight. In this study, the criterion of 1% of the specimen's weight has been used and it could fulfill the requirements of both the target porosity and the realistic contact force distribution. It should be noted that the value of the criterion could be smaller than 1% of the specimen's weight, but it will cause more iteration steps and increase the computation time. Moreover, if the value of the criterion is larger than 1% of the specimen's weight, the contact force distribution might not as rational as that in reality. Therefore, the criterion of 1% of the specimen's weight has been suggested. The relative displacement of the top plate was measured and the new 2D porosity could be calculated and compared with the initial 2D porosity. If the relative change of the 2D porosities was less than 0.005, the effect of porosity differences on the stress–strain relations of soil was quite small, especially for dense specimens according to the studies by Zeng (2006). Therefore, the effects can be neglect and the initial 2D porosity could be used for further DEM simulations. If not, the initial 2D porosity was changed correspondingly and new preliminary simulations were conducted with the changed 2D porosity again. The iterative process is shown in Fig. 3.

The contact force distribution with $n_{2D} = 0.14$ is shown in Fig. 5. The contact forces distribute all over the specimen. Moreover, the vertical force measured on both the top and the bottom plates were quite large ($F_{top} = 3854$ kN/m and $F_{bottom} = 3855$ kN/m), which were much larger than the self-weight of the specimen ($G_{specimen} = \rho_s \cdot (1 - n_{2D}) \cdot W \cdot H \cdot g = 846$ N/m). Hence, further steps were

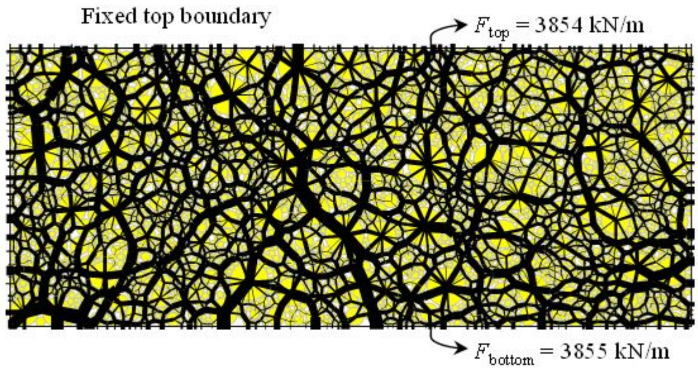


Fig. 5 Contact force distribution in the specimen with $n_{2D} = 0.14$, thickness of lines proportional to magnitude)

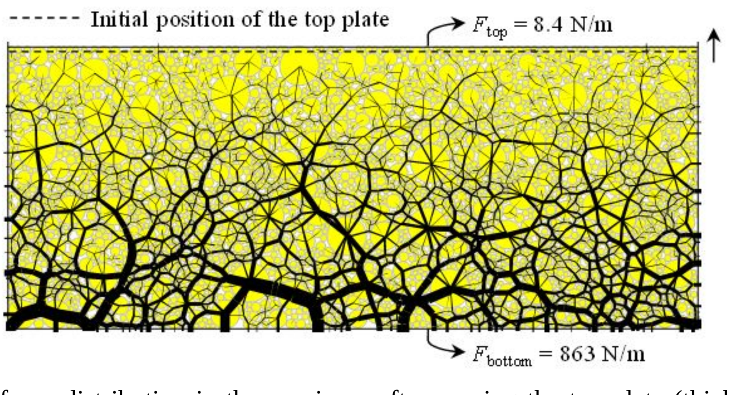


Fig. 6 Contact force distribution in the specimen after moving the top plate (thickness of lines proportional to magnitude)

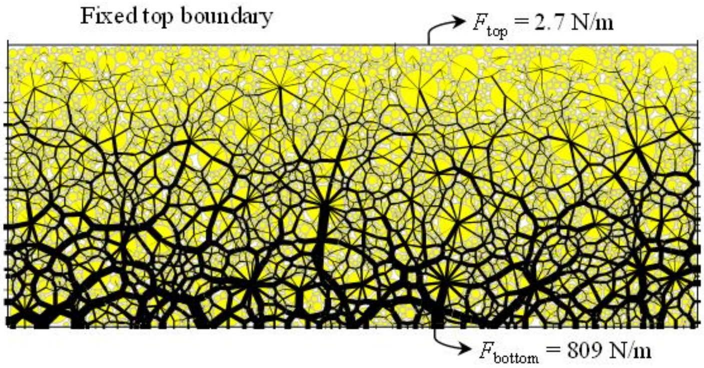


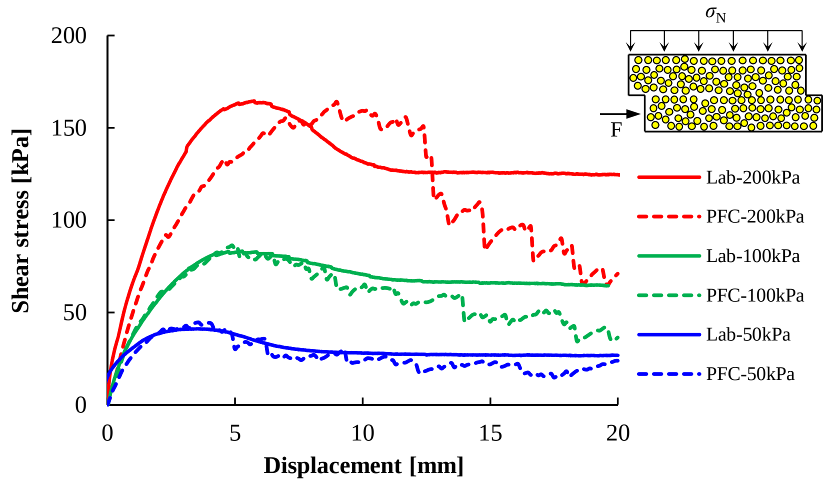
Fig. 7 Contact force distribution in the specimen with n_{2D} = 0.15 (thickness of lines proportional to magnitude)

conducted and the contact force distribution after moving the top plate is shown in Fig. 6. The contact force distribution in Fig. 6 is more realistic compared with that in Fig. 5, i.e., the contact forces were increasing with depth of the specimen under the gravitational load and the contact forces at the lower parts of the specimen were larger than those at the upper parts of the specimen. However, the relative change of the 2D porosities was 0.008, which was greater than the required value. Hence, further DEM simulations with a new 2D porosity were carried out.

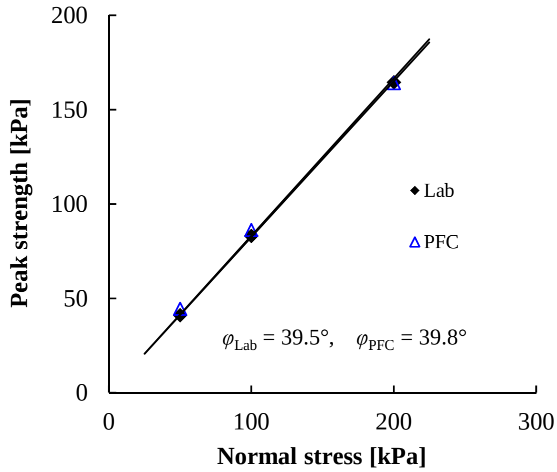
Fig. 7 shows the contact force distribution in the specimen with n_{2D} = 0.15, in which F_{top} meets the requirement of the criterion with a reasonable value of F_{top} = 2.7 N/m. The vertical force measured on the bottom plate was F_{bottom} = 809 N/m, which was quite close to the self-weight of the specimen ($G_{specimen} = \rho_s \cdot (1 - n_{2D,MLIM}) \cdot W \cdot H \cdot g$ = 836 N/m). Moreover, the contact force distribution was similar to the realistic contact force distribution under the gravitational load. Therefore, the selected 2D porosity of n_{2D} = 0.15 was regarded reasonable for conducting further DEM simulations in this case. The corresponding number of the soil particles was 2552 (n_{2D} = 0.15).

4. Further DEM simulations

In order to verify the new 2D porosity is also applicable for further DEM simulations, both experimental and numerical direct shear tests have been carried out with the normal stresses of 50, 100 and 200 kPa. The experimental direct shear tests were conducted using the large-scale direct shear apparatus ($W/D/H$ = 305 /305 /124 mm^3) at the geotechnical laboratory of RWTH Aachen University. In those tests, dry sand with the particle size distribution in Fig. 4 has been used and the specimens were prepared with four layers by compacting each layer to the target testing porosity of 0.3434 and the corresponding density was 1.74 g/cm^3. During the shearing process, a fixed shear rate of 0.384 mm/min was applied, while the normal stress applied on the top of the specimen was kept constant. For DEM simulations, the main micro input parameters are listed in Table 1. The testing 2D porosity was 0.15 and the shear rate was also 0.384 mm/min. Detailed information about the numerical direct shear tests can be found in Wang *et al*. (2014). Fig. 8 compares the DEM simulation results with the corresponding experimental data. Although there are some differences on the shear stress–displacement relations between the laboratory tests and



(a) Shear stress–displacement relations



(b) Peak strength–normal stress relations

Fig. 8 Comparison of the experimental and numerical direct shear tests

the DEM simulations in Fig. 8(a), the internal friction angle obtained from the peak strength-normal stress relations based on the DEM simulations has shown good agreement with that based on the laboratory tests (Fig. 8(b)).

Together with the reasonable contact force distribution in the specimen in Fig. 7, it can be concluded that the parabolic equation and the criterion suggested in this study can be used as a guideline to determine 2D porosities for DEM studies.

5. Discussion

The shapes of the soil particles in practice are various, which makes the investigations with real particle shapes extremely difficult (Jumikis 1962). Therefore, many studies have been conducted on particles with circular or spherical shapes (Nicot *et al*. 2007, Wang and Leung 2008, Bhandari and Han 2010, Mohamed and Gutierrez 2010, Jiang *et al*. 2011, Han *et al*. 2012, Tran *et al*. 2013, Bhandari *et al*. 2014). In this study, all the particles were assumed to have circular shapes and large friction coefficients have been used so as to compensate the lack of angularity of circular particles.

As it is shown in Fig. 5, large contact forces existed in the specimen without any normal stresses on the top of the specimen (n_{2D} = 0.14). In order to reduce the large contact forces without changing the target 2D porosity, the unique way is to decrease the contact stiffnesses of the particles and the walls since the friction coefficient of the particles for the specimen preparation was already very low according to Härtl and Ooi (2008). However, it is a general rule that the initial Young's modulus of the material is linearly related to the value of the contact stiffness (Itasca 2008), i.e., the contact stiffness should be adjusted to accord with the experimental data after the specimen generation. Therefore, the large contact forces in the specimen at the initial stage might be caused by the unreasonable 2D porosity. The parabolic equation provides a general relation between 2D and 3D porosities, which can be used as a rough guideline to adjust the 2D porosities so as to rapidly meet the requirements of the criterion for a wide range of polydisperse particle systems.

Fig. 7 shows a realistic contact force distribution in the specimen, in which the contact forces at the lower parts are larger than those at the upper parts. It represents that the 2D porosity obtained based on the parabolic equation and the criterion in this study is reasonable. Moreover, after fixing the 2D porosity, further DEM simulations have been conducted by calibrating the contact stiffnesses and the friction coefficients of the particles and walls with the experimental direct shear test results. Fig. 8 shows good agreement of the DEM simulation results with the experimental data. It should be noted that the final input parameters used in further DEM simulations in this study also meet the requirements of the realistic contact force distribution in the specimen.

The suggestion for the determination of 2D porosities has been satisfactorily verified with dense specimens (relative density D_r = 0.89) in this study. The verification of the criterion for medium dense and loose granular material is still needed to be proved.

6. Conclusions

In this study, different approaches for converting porosities from 3D to 2D have been summarized and theoretically evaluated. A parabolic equation and a criterion have been suggested for the determination of 2D porosities in DEM studies. The following conclusions can be drawn:

- The current approaches tried to link the 2D and 3D porosities just using specific equations, which might be impossible for arbitrary assemblies with various polydisperse particle systems.
- The parabolic equation and the criterion in this study provide a simple yet reasonable method to select an appropriate 2D porosity, which meets the requirement of both the realistic contact force distribution in the specimen and the good agreement of further DEM simulation results with the corresponding experimental data. Therefore, the parabolic equation and the criterion are suggested for the determination of 2D porosities in a wide range of polydisperse particle systems.

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