DEM simulation of liquefaction for cohesionless media at grain scale

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Abstract: Simulations of undrained tests were performed in a periodic cell using three dimensional (3D) discrete element method (DEM) program TRUBAL. The effective undrained stress paths are shown to be qualitatively similar to published physical experimental results of cohesionless media such as sand. Liquefaction and temporary liquefaction are observed for very loose samples and medium loose samples, respectively. A new micromechanical parameter is proposed to identify whether liquefaction or temporary liquefaction occurs in terms of a redundancy factor. The relationship of redundancy factor and average coordination number is derived theoretically. It is demonstrated that the phase transition dividing the solid-like behaviour and liquid-like behaviour is associated with a redundancy factor of 1, which corresponds to an average coordination number slightly above 4.

Key words: simulation; discrete element; TRUBAL; liquefaction; redundancy factor; coordination number

1 Introduction

Since the pioneering work of BISHOP [1–2] and CASTRO [3], many researchers have conducted investigation of undrained behaviour especially for loose sand. POULOS [4] defined and explained the concept of steady state (SS) deformation for any mass of particles, which corresponds to a state in which the mass continuously deforms at constant volume, constant normal effective stress, constant shear stress, and constant velocity. ALARCON-GUZMAN et al [5] defined a quasi-steady state (QSS), where a ‘steady’ state is temporarily held but deviator stress goes up further with strain. ISHIHARA et al [6] called QSS a phase transformation (PT) state because it defines a transition from contractive to dilative behaviour. Corresponding to steady state, liquefaction is said to occur. Corresponding to quasi-steady state, limited (partial, temporary) liquefaction is said to occur. There has been some argument about whether the quasi-steady state is a real material behaviour. BEEN et al [7] suggested that the quasi-steady state could be a real material property. WANG [10] pointed out that liquefaction can attribute to sand boil, flow slide (monotonic shear loading) and cyclic mobility, and investigated the mechanism of soil liquefaction under different loading conditions.

Although the undrained behaviour (such as liquefaction) has been studied experimentally by many researchers, the concept has not been well explored at grain or microscopic level. This may be due to the fact that the traditional analysis of the undrained response in the past was based on continuum concept. The discrete element method (DEM) provides an ideal tool to examine the behaviour of granular materials such as sand at both macroscopic and microscopic levels. Furthermore, DEM can provide exactly the same initial sample repetitively, which is impossible in the laboratory physical tests. In DEM, a sample consists of discrete particles, which only interact at particle contacts. The particles can rotate, slide and separate. With such a system, DEM is particularly suitable for modeling granular material behaviour or structures with discontinuous features. DEM was originally developed by CUNDALL [11] for the analysis of rock mechanics problems. CUNDALL and STRACK [12] published the first journal paper on DEM, and they studied soil behaviour using 2D DEM program BALL. CUNDALL [13] introduced 3D DEM program TRUBAL, and
periodic cell was incorporated in TRUBAL. A periodic cell allows a particle that moves out of the cell to be re-mapped back into the cell at a corresponding location on the opposite face. The particle that moves out of the cell carries all the same information as that moving into the cell, except for particle positions. An infinite lattice can be imagined by replicating one cell throughout space. Thus, the simulation can be performed free from boundaries. CUNDALL [14] predicted a discontinuous future for numerical modeling in geomechanics. In this work, a new microscopic parameter in terms of redundancy factor is proposed to describe liquefaction for cohesionless media, and the evolution of redundancy factor is provided using DEM simulations under undrained conventional triaxial conditions.

Most DEM simulations are performed ‘in a vacuum’ without fluid, as done in this work. However, in principle, it is necessary (especially for undrained conditions for partially-saturated samples) to model the fluid phase and how the fluid/particle phases interact with each other, e.g. in DEM simulations of fluidised beds [15−17] in order to obtain complete information. In the DEM simulations reported in this work, the fluid phase is ignored and all stresses are calculated from the orientational distributions of forces at the contacts between particles. Consequently, the effective stresses are calculated directly. This is in contrast to laboratory experiments in which the total stresses and the pore water pressure are measured and the effective stresses are obtained indirectly using Terzaghi’s effective stress equation.

However, constant volume conditions are only suitable for mimicking undrained condition for saturated samples. The undrained behaviour was modelled using 2D DEM by THORNTON and BARNES [18], NG and DORBY [19], ZHANG [20], BONILLA [21] and SHAFIPOUR and SOROUS [22]. Most of these researchers used 2D constant volume simulations for mimicking undrained saturated soil tests, except that BONILLA [21] and SHAFIPOUR and SOROUS [22] used both constant volume and coupled fluid–particle interaction methods. The comparison of undrained behaviour using constant volume and fluid–particle interaction methods showed no difference essentially as indicated by BONILLA [21] and SHAFIPOUR and SOROUS [22]. It is difficult to say whether 2D undrained biaxial situation can represent 3D conditions, since the degree of freedom of 2D particle and that of 3D particle are different. SITHARAM et al [23] presented 3D undrained (constant volume) simulation results under axisymmetric compression for very loose samples. Of all the above researchers, only BONILLA [21] and SHAFIPOUR and SOROUS [22] observed temporary liquefaction in their DEM simulations.

2 Simulation details

Three-dimensional DEM simulations have been performed on polydisperse systems of 3 600 elastic spheres using the same TRUBAL code as used by THORNTON [24]. Contact interactions are calculated using algorithms based on the theories of HERTZ (normal interaction) and MINDLIN and DERESIEWICZ [25] (tangential interaction) (see also Refs. [26−27]). The elastic modulus and Poisson ratio for each particle were specified as $E=70$ GPa and $\nu=0.3$, respectively. During the shear stage, the interparticle friction coefficient was set to be $\mu=0.5$. Nine different sizes of spheres were used: 0.25 mm (2), 0.26 mm (20), 0.27 mm (220), 0.28 mm (870), 0.29 mm (1376), 0.30 mm (870), 0.31 mm (220), 0.32 mm (20) and 0.33 mm (2), with an average particle diameter of 0.29 mm (the actual number of particles is given in brackets). The notional density of each particle is $2\text{ 650 kg/m}^3$, which is scaled up by a factor of $5 \times 10^12$ in order to perform quasi-static simulations within a reasonable timescale. Such density scaling does not affect the quasi-static stress–strain behaviour [24]. The time step used in the simulations is based on the minimum particle size and the Rayleigh wave speed [28]. CUNDALL and STRACK [12] introduced global and contact damping in order to dissipate sufficient kinetic energy. In the DEM simulations presented in this work, only contact damping is used. No gravity field is applied and cohesion is set to be zero.

Sample preparation for DEM is a time-consuming process. In order to achieve a system which could be used for subsequent shear simulations, isotropic compression with servo control [24] was carried out in stages by incrementally increasing the stress level until an isotropic stress of 100 kPa was obtained. The inter-particle friction was adjusted during the early isotropic compression stage until the isotropic stress was nearly 100 kPa, and the inter-particle friction coefficient was then changed to 0.5. In order to obtain the loosest sample, particle rotations were prevented during the early isotropic compression stage. Without particle rotation, the assembly is stiffer and more resistant to isotropic compression. Particle rotation was then permitted during the later stages of isotropic compression and shear stages. In this way, the loosest sample (porosity $n=0.425$) was prepared. In total, six loose samples were prepared with porosities ranging from 0.405 to 0.425. More details are provided in Ref. [29].

All the undrained simulations reported were carried out in a periodic cell in order to eliminate any boundary effects. To mimic undrained tests, the constant volume condition was simulated in which the initial strain rates in the three principal strain directions were set to be
1.0×10⁻² s⁻¹ (compression), −5.0×10⁻³ s⁻¹ and −5.0×10⁻⁵ s⁻¹ (extension), respectively. All the simulations start from an initial stress state that is almost isotropic with all the normal (principal) stresses approximately equal to 100 kPa.

During the simulations, the ensemble average stress tensor is calculated (see also Ref. [30]) as follows:

\[
<\sigma_{ij}> = \frac{1}{V} \sum_{i=1}^{C} [(R_i + R_2)N_i n_j + (R_i + R_2)T_i t_j]
\]  

(1)

where the summations are over the C contacts in the volume V; \( R_1 \) and \( R_2 \) are the radii of the two spheres in contact; \( N \) and \( T \) are the magnitudes of the normal and tangential contact forces at the contact; \( n \) is the unit vector normal to the contact plane and \( t \) is the unit vector parallel to the contact plane.

The average coordination number \( Z_a \) is calculated as follows (see also Ref. [31]):

\[
Z_a = \frac{2C}{N_p}
\]  

(2)

where \( C \) is the number of contacts and \( N_p \) is the number of particles.

3 Results and discussion

The results are presented of undrained test simulations on all the loose samples and both the macroscopic and microscopic behaviours are discussed. The macroscopic behaviour is presented in terms of stress path and evolution of deviator stress. The microscopic behaviour is presented in terms of average coordination number and redundancy factor.

3.1 Macroscopic behavior

Figure 1 shows the undrained (constant volume) stress paths in terms of deviator stress \( q (q=\sigma_1-\sigma_3) \) against mean effective stress \( p' (p'=(\sigma_1+\sigma_2+\sigma_3)/3) \) for the six samples under undrained axisymmetric compression (UAC) condition. Figure 2 shows the deviator stress \( q \) plotted against deviator strain \( (\varepsilon_{dev}=\varepsilon_1-\varepsilon_3) \) for all the systems. The initial state on the stress path is the isotropic stress point \((p'=100 \text{ kPa}, q=0)\). It can be seen from both the figures that for all the very loose samples (porosity \( n=0.425, n=0.419 \) and \( n=0.414 \)), the deviator stress increases to an initial peak, followed by a decrease to a minimum value, and with further straining, \( q \) does not go up, which corresponds to steady state (SS) or liquefaction in soil mechanics as mentioned in Section 1. The medium loose samples (porosity \( n=0.409, n=0.407 \) and \( n=0.405 \)) exhibit similar behavior as very loose samples, but the initial peak of \( q \) is larger and there is obvious increase of \( q \) after the minimum value is obtained, which corresponds to quasi-steady state (QSS) or temporary liquefaction as mentioned in Section 1. The sample \( n=0.405 \) exhibits much larger minimum value of \( q \) than other samples, the sample exhibits very short temporary liquefaction behavior, and as pointed out later in Subsection 3.2, a microscopic explanation to this is provided. Figure 1 indicates that all the samples reach a unique line passing through the origin at final stages in stress path, called ultimate state line, which means that the slope \((M=q/p')\) of the ultimate state line is constant. The relationship between \( M \) and \( \sin \phi \) for undrained axisymmetric compression is \( M=6\sin \phi/(3-\sin \phi) \), where \( \sin \phi=(\sigma_1-\sigma_3)/2(\sigma_1+\sigma_3) \) and \( \phi \) is called mobilized friction angle. Figure 1 seems to imply that \( M \) is independent of porosity. The value of \( M \) (about 0.77) in these undrained simulations is very close to the critical state value (0.74) in drained constant mean stress simulations from Ref. [29]. The experimental finding by BEEN et al [7] indicates that \( M \) at steady state under undrained condition is the same as the value of \( M \) at critical state under drained condition, which agrees with the DEM simulation results in this work. Typical \( M \) values at
steady state from different researchers are listed in Table 1, where it can be seen that the $M$ value at steady state in the DEM simulation presented in this work is smaller than other typical values. This is due to the fact that the particle shape adopted in this DEM simulation is spherical, which leads to more feasibility for particle rotation thus causing a lower steady state strength. However, the value of 0.77 is reasonably close to that from Ref. [7], which at least qualitatively validates these DEM simulation results. It can be seen from Fig. 2 that the minimum values of $q$ at SS for the very loose samples are not exactly zero ($q=2$ kPa for $n=0.425$). YAMAMURO and LADE [33], among others, defined static liquefaction as a special case of steady state with zero effective confining pressure and zero deviator stress. However, even in the liquefied state, there exist interparticle collisions (as shown later) leading to a state of stress that is never actually zero but simply a rather small value in the context of traditional soil mechanics.

<table>
<thead>
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<th>Table 1</th>
<th>$M$ values of typical sand at steady state under undrained conditions</th>
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It can be concluded from Fig. 2 that the initial peak of $q$, the $q$ value at SS and the $q$ value at OSS all depend on the porosity of sample, decreasing with the increase of porosity. Consequently, liquefaction resistance decreases as porosity increases. This is in agreement with traditional experimental observations.

3.2 Microscopic behavior

The coordination number is related to the stability of the structural system [24, 34]. Consider a 3D assembly with interparticle friction $\mu=\infty$, i.e. no sliding anywhere. The number of degrees of freedom of a single particle is six (three rotations and three translations), so the total number of degrees of freedom in the system is $6N_p$, where $N_p$ is the number of particles. The number of constraints (unknown forces) at a contact is three (one normal constraint and two tangential constraints), so the total number of constraints in the system is $3C$, where $C$ is the number of contacts. If the system is statically determinate, a limit condition is $3C=6N_p$ and then the limit coordination number $Z_n=2C/N_p=4$. If the system is statically indeterminate, i.e. having more contacts than necessary to satisfy equilibrium, then $Z_n>4$ and in this case the macroscopic behaviour can be said to be ‘solid-like’. If $Z_n<4$, the system is unstable and the system becomes a structural mechanism, which can lead to further loss of contacts with the consequence that the macroscopic behaviour can be said to be ‘liquid-like’.

Figure 3 shows the average coordination number, defined by Eq. (1), plotted against deviator strain for all the systems. It can be seen that the average coordination number decreases initially for all the loose systems until a minimum value is reached. However, even at steady state when liquefaction occurs, the minimum value of $Z_n$ is about 0.5 (>0) for the loosest sample, therefore particle collisions exist, causing the deviator stress at steady state (or residual strength) to be greater than 0 (the actual value of residual strength for the loosest sample is about 2 kPa). It can be seen that given a fixed value of deviator strain except for the initial shear stages at very small strains, the value of $Z_n$ is dependent on the porosity, decreasing with the increase of porosity. From the definition of $Z_n$ from Eq. (2), as the number of particles is fixed at 3 600, the evolution of average coordination number actually represents the evolution of number of contacts, which is important for the stability of the particulate system. If a system has more contacts, it will generally be more stable and more resistant to liquefaction/temporary liquefaction. Therefore, liquefaction resistance decreases as porosity increases. This explains the macroscopic observations discussed in Subsection 3.1.

![Fig. 3 Evolution of average coordination number under UAC](image-url)
Fig. 4 Evolution of redundancy factor under UAC

Reduced number of constraints at contacts where sliding occurs) to the number of degrees of freedom in the system. In 3D systems, a sliding contact is associated with loss of two tangential constraints, therefore,

\[ F_R = \frac{C}{N} \left( \frac{3-2f}{6} \right) = Z_a \left( \frac{3-2f}{12} \right) \]  

(3)

where \( f \) is the fraction of sliding contacts, e.g. 0.10. If \( F_R > 1 \), then we have a redundant system and the system can be said to be solid-like, and for \( F_R < 1 \) we have a structural mechanism and the system can be said to be liquid-like. Therefore, \( F_R = 1 \) defines a limit phase transition line from solid-like to liquid-like behavior.

Figure 4 shows the evolution of redundancy factor, defined by Eq. (3), under UAC for all the systems. It can be seen that a phase transition line, defined by \( F_R = 1 \), clearly divides the solid-like region and liquid-like region. Below the phase transition line, the system is in liquefied or temporarily liquefied state. Above the phase transition line, the system is in stable non-liquefied state. The phase transition indicates the onset of liquefaction or temporary liquefaction. It can be easily seen that the phase transition (the onset of liquefaction or temporary liquefaction) occurs at very small strain for the loosest sample, and occurs at relatively larger strain for denser samples. It can be seen that the three very loose samples do not re-establish solid-like behavior after the phase transition. The two medium-loose samples (\( n = 0.409 \) and \( n = 0.407 \)) get close to phase transition line within the simulated strain ranges. The medium-loose sample (\( n = 0.405 \)) re-establish solid-like behavior quickly after phase transition, and can be considered to be generally solid-like during the whole undrained process. GONG [29] found that all the samples reported in this work converge to a unique porosity of 0.407 at critical state (see Ref. [35]) at drained simulation with constant mean stress of 100 kPa. Therefore, it can be deduced from the above observations that when the porosity of a saturated sample is greater than the corresponding critical state porosity under drained condition, the sample will generally have a solid-like behavior during the process of undrained conditions.

For comparison, the evolution of redundancy factor under drained constant mean stress of 100 kPa (the simulations were reported in Ref. [29]) is reproduced in Fig. 5. It can be seen that all the samples exhibit solid-like behaviour \((F_R > 1 \text{ always})\) under drained condition, which means that the samples do not liquefy under drained condition. This agrees with the common sense for the macroscopic behaviour of loose saturated samples under drained conditions.

Fig. 5 Evolution of redundancy factor under drained constant mean stress of 100 kPa

Equation (3) provides a relationship between the redundancy factor and average coordination number. It should be noted that the relationship depends on the fraction of sliding contacts, which differs from sample to sample. However, GONG [29] showed that the fraction of sliding contacts is always smaller than 0.1 at any stage. Therefore, the relationship between the average coordination number and the redundancy factor is almost unique independent of the porosity of samples, as demonstrated in Fig. 6(a). It can be seen that the average coordination number associated with the phase transition \((F_R = 1)\) is a little above 4. As derived previously, the limited average coordination number is 4 when interparticle friction coefficient \( \mu = \infty \). As \( \mu \) becomes finite or smaller, there will be more contacts required to keep the system stable, and consequently the limit average coordination number will become larger. However, Fig. 6(a) indicates that an average coordination of 4 should be a good approximation of phase transition (or limited \( Z_a \)), and actually can act as a lower bound for the limit \( Z_a \) when \( \mu \) is finite. Figure 6(b) shows clearer correlation between average coordination number and redundancy factor with the value of \( F_R \) between 0.9 and 1.1.
Fig. 6 Correlation between average coordination number and redundancy factor: (a) $F_R=0$–1.4; (b) $F_R=0.9$–1.1

4 Conclusions

1) A microscopic parameter redundancy factor $F_R$ is introduced to define the phase transition from solid-like to liquid-like behaviour and the onset of liquefaction. And the limit phase transition is found to be associated with a redundancy factor of 1.

2) An average coordination number of 4 can be taken as a lower bound for limit phase transition to occur when interparticle friction coefficient is finite.

3) The liquefaction of very loose samples, and temporary liquefaction of medium-loose sample under undrained axisymmetric compression condition are well captured at macroscopic level at least qualitatively, using 3D DEM simulations. And the microscopic information captured by the DEM simulations provides a rational explanation to the macroscopic behaviour.

Acknowledgements

The authors would like to thank Prof. Andrew Chan and Dr. Colin Thornton, both from University of Birmingham, UK, for their guidance and discussion on the relevant work.

References


