ABSTRACT: This paper highlights the potential of Discrete Element Method (DEM) simulations to capture the cyclic behavior of the granular materials including liquefaction, post liquefaction and dynamic properties. A series of strain controlled undrained cyclic triaxial tests have been carried out on isotropically compressed assembly of spheres to understand the influence of different parameters on the cyclic behavior of granular materials. The undrained tests have been simulated by maintaining a constant volume condition of the sample throughout the cyclic triaxial tests. Post liquefaction undrained monotonic studies were carried out on samples without dissipating the excess pore water pressure developed during initial liquefaction. As observed from the results, numerical simulation using DEM has captured liquefaction, pore water pressure generation, post-liquefaction and dynamic properties similar to the experimental results. Furthermore, evolution of micromechanical parameters such as average coordination number and anisotropic coefficients during cyclic triaxial loading has also been reported and discussed.

INTRODUCTION
For the last few decades, the behaviour of saturated granular materials during undrained cyclic loading condition has attracted the attention of researchers worldwide. The high incidence of liquefaction during earthquakes, with its potential to damage, has made the liquefaction a prime subject of concern in geotechnical earthquake engineering. It has been reported, based on the laboratory investigations, that liquefaction and pore water pressure response during cyclic loading depends on many factors such as confining pressure, initial void ratio, initial stress condition, amount of fines, sample preparation method, over consolidation ratio, length of time under sustained pressures [1-9]. Despite the extensive research in this area, liquefaction still remains a major problem even in recent earthquakes. This is due to the fact that the mechanical behaviour of granular materials is influenced by a large number of factors, which make it difficult to establish general stress – strain relationships.

The major concern during earthquake loading was to safe guard the structure from liquefaction, if the structures are resting on saturated loose sand. Often, costly ground improvement projects (e.g. densification of sand) are preferred to mitigate the liquefaction hazards (e.g. earthquake induced displacements). In the last two decades, the need for evaluating earthquake-induced settlements was recognized and as a result, some analytical and empirical relationships were developed [10-12]. The important information required to evaluate the earthquake induced displacement is the undrained stress-strain response of the post liquefied sands. This will allow the designer to predict the potential resistance of liquefied sand to withstand the monotonically increasing static loads. This information is also required for the assessment of post liquefaction stress strain behaviour of soils to mitigate liquefaction hazards. Recent laboratory investigations [13-15] have achieved a qualitative understanding from laboratory investigation on the post liquefaction undrained behaviour of sandy soils. However, no attempt has been done so far to understand the post liquefaction monotonic undrained test from grain scale level.

The behaviour of soils subjected to dynamic loading is governed by dynamic soil properties. The measurement of dynamic soil properties is critical task in the solution of earthquake geotechnical engineering program. Since dynamic properties are influenced by several factors, precise measurement of dynamic soil properties is somewhat a difficult task in the solution of geotechnical earthquake engineering problems [16]. Several laboratory and field techniques are available to measure the dynamic properties of soils. Some of these tests are oriented toward measurements of dynamic properties at low strain levels and some other towards large strain levels. However it is highly difficult to determine the dynamic properties for wide range of shear strain level (from low shear strain to high) using single testing apparatus. Moreover, in the recent past, many experimental investigations mostly for sandy soil have been carried out to investigate the effect of parameters such as confining pressure, amplitude of shear strain, void ratio, number of cycles, stress history, initial stress, soil type etc on the dynamic properties [17-20]. These experimental investigations are mostly confined to isotropically consolidated samples without considering the initial soil structure or fabric. Since dynamic properties are highly sensitive to all these factors it is highly essential to evaluate these properties using a numerical technique which can model granular material as an assemblage of particles for wide range of shear strain where in sample preparation problem can be avoided.

To comprehensively understand the macroscopic behavior of granular materials an understanding of the micromechanical response during cyclic loading is necessary. This approach requires observations at micro level, which is very difficult to achieve by actual experiments on real granular media. This
can be easily achieved by particulate modeling approaches. In this direction, early attempts to observe force distributions and particle behaviour at microscopic levels were made by Dantu [21] and Wakabayashi [22] using optically sensitive materials. Later, De Josselin de Jong and Verruijt [23] analyzed force distribution in such assemblies, studying individual particles. The results of these experiments provided a qualitative understanding of the mechanisms of load transfer and the deformation characteristics of granular materials. New experimental techniques [24] using computer tomography also provide important information about the evolution of the fabric. However, these analytical models were applicable only for regular arrays of spheres and discs of uniform size under simple loading. These tests are expensive and time consuming also the data is insufficient for micromechanical analysis. A way out of this difficulty is computer simulated numerical experiments which offers complete information of all microscopic features for detailed analysis. One such numerical technique is by using Discrete Element Method (DEM) pioneered by Cundall and Strack [25]. DEM models the soil as discrete particles interacting through contact forces without any assumptions of continuum, isotropy and the macro behavior is obtained from micro response at the contacts. An accurate measurement of contact forces and displacement is possible and also sufficient micro-parameters data can be extracted for micromechanical analysis.

In this study, DEM modelling has been used to simulate the liquefaction, pore pressure response, post-liquefaction undrained monotonic behaviour and dynamic soil properties of granular materials. The macroscopic results for all the numerical simulations are presented along with micromechanical explanations in terms of average coordination number and deviator anisotropic coefficients. The aim is to have an insight into the internal fabric and microscopic behaviour so as to bridge the gap in the understanding of the macro behaviour from micro response.

**DISCRETE ELEMENT METHOD**

Discrete Element Modelling (DEM) is pioneered by Cundall and Strack [25], which employs an explicit finite difference scheme. The fundamental idea of DEM is that each particle is modeled as an element obeying Newton’s second law of motion. Equilibrium contact forces and displacements are found in a stressed assembly of particles through a series of calculations tracing the movement of each particle. The movement of each particle is tracked by solving a set of Newton’s equation of motion. A contact force generates when the elements overlap and the magnitude of contact force is determined by the force-displacement law. Coulomb’s friction law is adopted for the relative slippage between elements. A suitable damping in the form of Rayleigh damping is incorporated to dissipate the kinetic energy generated. The resultant force vector on each element is the vectorial sum of contact forces. The law of motion is applied to each sphere during the time step. The particle accelerations, velocities and displacements are obtained by integrating the law of motion and are assumed to be constant over a time step. During the next time step, new set of contact forces on a sphere particle is obtained from force-displacement law and the cycle of calculation will continue. Force boundary conditions, displacement boundary conditions and gravitational loads can be applied on the system. A typical calculation cyclic is shown in Fig. 1. In DEM, internal stresses and contact behavior can be captured efficiently, and sample reproducibility is guaranteed. The major advantage is the wealth of micromechanical and statistical information that can be generated by the DEM simulations along with the macroscopic response.

**NUMERICAL SIMULATION PROGRAM**

DEM simulations have been carried out using TRUBAL (3 D version) modified by incorporating (1) subroutines to extract the micro and macro parameters, (2) post processors for program developed using JAVA [26-28]. In this study, an assembly of 1000 spheres having particle sizes varying from 0.2 to 2 mm has been considered. Linear force displacement contact model was employed for the numerical simulation programme. Particle stiffness of the spherical particles in the linear contact model was evaluated by assuming the same strain (δ/d) for both Hertzian and linear contact model [28, 29]. Fig. 2 shows the initially generated assembly without any overlap in a cubic space having periodic space boundary. These sphere particles were assigned a Young’s modulus of 70 GPa; Poisson’s ratio of 0.3; density of 2650 kg/m³ and a contact friction value of 0.5. After generation, the assembly was compacted isotropically using a strain rate of 10⁻⁴/s to a desired initial confining pressure. A series of undrained strain controlled cyclic triaxial numerical simulations have been carried out on isotropically compressed samples at a frequency of 1.42 Hz. Undrained tests in the present investigation have been carried out by keeping the volume constant throughout the shearing process. After initial liquefaction, which is defined as the state at which the pore water pressure builds up to a value equal to the initially applied confining pressure, undrained monotonic tests were carried out on samples without dissipating the excess pore water pressure developed during initial liquefaction.
RESULTS AND DISCUSSIONS

DEM simulation results were expressed using macroscopic stress parameters such as deviator stress \(q\) and mean \(p\) (in undrained test effective stresses are used to calculate \(p'\)) which are defined as follows:

\[
p = \frac{\sigma_{11} + 2\sigma_{33}}{3} \tag{1}
\]

\[
q = \sigma_{11} - \sigma_{33} \tag{2}
\]

In granular materials, forces are typically carried by the contacts between the particles. Hence, quantifying the arrangement of contacts is quite essential in understanding the load-carrying capacity of granular materials. To quantify these, microstructure features Rothenburg and Bathurst [30], Chantawarangul [26] and Sitharam et al. [31] introduced parameters such as anisotropy coefficients in contact orientation, average contact force, and tangential contact force.

\[
\begin{align*}
    a_{ij}^{p} &= \frac{3}{2} a_{ij}^{p} a_{ij}^{p} + a_{ij}^{p} \\
    a_{ij}^{n} &= \frac{3}{2} a_{ij}^{n} a_{ij}^{n} + a_{ij}^{n} \\
    a_{ij}^{t} &= \frac{3}{2} a_{ij}^{t} a_{ij}^{t} + a_{ij}^{t}
\end{align*} \tag{3}
\]

Where \(a_{ij}^{p}\), \(a_{ij}^{n}\), and \(a_{ij}^{t}\) are the symmetric second order deviatoric tensor representing coefficient of fabric anisotropy, normal contact force anisotropy and tangential contact force anisotropy. More details regarding the micromechanical parameters and the development of stress-force-fabric relationship can be found elsewhere (eg. Chantawarangul, 1993; Sitharam et al. 2002 and Sitharam and Vinod, 2008).

Liquefaction and pore water pressure response

Figure 3 presents the variation of deviator stress and excess pore water pressure ratio with number of cycles for a confining pressure of 100 kPa [29]. Figure 4 shows the plot of average coordination number with mean \(p'\) during cyclic loading. The average coordination number, \(Z = M/N\), of the assembly is defined as the ratio of total number of contact points \(M\) within the assembly volume \(V\) to the total number of particles \(N\) in the assembly. A steady decrease in the average coordination number with decrease in the mean \(p'\) can be observed from Fig. 4. This steady decrease in the average coordination number is due to the development of excess pore pressure during constant cyclic strain loading in undrained condition. The average coordination number drastically decreases at a value close to 3 which corresponds to the collapse of the soil structure.

Combined analysis of shear strain (%) and number of cycles for liquefaction for the range of void ratio and confining pressure considered for the study is presented in Fig 5. The numerical simulation results are also compared with the strain controlled laboratory experimental results carried out by Talaganov [7] and GovindaRaju [32]. It is evident that there exists a unique relationship between shear strain and number of cycles for initial liquefaction for the range of void ratio and confining pressure considered for the study.
Moreover it is apparent that the numerical simulation results falls close to the laboratory experimental investigations. Also presented in this figure the lower and upper bound proposed for sands by Dobry [33] from the strain controlled laboratory experiments for comparison. It is evident that excess pore water pressure generation can be predicted accurately from the shear strain amplitudes. All the DEM results irrespective of initial confining pressure, void ratio and amplitude of strain falls close to the lower bound curve for sands [33].

Post liquefaction Results

Figure 7 shows the results of post liquefaction undrained monotonic response of sand samples liquefied at different axial strain amplitude (ε = 0.3%, 0.5% & 0.6%) for a confining pressure of 100 kPa prior to initial liquefaction. It is seen from Fig.7 that there is a pronounced influence of cyclic strain amplitudes on the post liquefaction monotonic strength of sands. All the samples exhibit an initial deformation with zero deviator stress up to a particular value of negative pore water pressure. Moreover, rate of increase of post liquefaction monotonic strength increases with decrease in the cyclic strain amplitudes. This may be due to the effect of cyclic strains on the soil fabric at liquefaction. During undrained monotonic loading on the liquefied samples, the deformation required to form a completely new soil fabric arrangement and to carry the deviator stress increases with increase in the amplitude of axial strain prior to liquefaction. Similar laboratory results have been reported by Vaid and Thomas [14] and Kukusho et al. [15].

Figure 8 presents the variation of average coordination number with axial strain at a confining pressure of 100 kPa for different amplitude of axial strain prior to initial liquefaction. It can be observed that the rate of building up of average coordination number during monotonic loading depends on the amplitude of axial strain applied prior to liquefaction. It is evident that the rate of building up of average coordination number increases with decrease in the amplitude of axial strain prior to liquefaction. The average coordination number steadily increases from zero (point of liquefaction) to a value of 4 and thereafter remains constant. Figure 9 shows the variation of deviator anisotropic coefficient with axial strain during monotonic undrained loading for a confining pressure of 100 kPa and axial strain amplitude of 0.6 % prior to liquefaction. Also shown in this figure is the variation of stress ratio with axial strain. It shows the influence of anisotropic coefficient on the development of post liquefied monotonic strength. A sudden increase in deviator anisotropic coefficients soon after the application of axial strain can be observed. Deviator coefficients show an oscillatory trend up to an axial strain of 3% due to the absence of particle contacts at the point of liquefaction. However, all the curves seems to stabilize beyond an axial strain of 3%. In addition, it can also be observed that the deviator coefficient of fabric dominates the normal contact force anisotropy at the point of liquefaction. With the
increase in the axial strain, it can be observed that there is a sharp decrease in the deviator normal contact force anisotropy and deviator coefficient of fabric up to an axial strain of 3%. Thereafter, the deviator normal contact force anisotropy dominates the deviator coefficient of fabric, which is reflected in the increase in deviator stress. Deviator tangential contact force anisotropy initially having a value close to 1 drops to a value of 0.1 with increase in axial strain, beyond which it remains constant with increase in axial strain during monotonic tests.

Fig. 8: Plot of average coordination number versus axial strain for different amplitude of axial strain prior to liquefaction [29].

![Graph showing average coordination number vs. axial strain](image1)

Fig. 9: Variation of deviator anisotropic coefficients and stress ratio with axial strain [29].

![Graph showing deviator anisotropic coefficients and stress ratio vs. axial strain](image2)

Comparison with assembly after dissipating the excess pore water pressure developed during initial liquefaction

Figure 10 presents the plot of stress ratio versus axial strain for samples with and without dissipating the excess pore water pressure during cyclic loading. A steady increase in stress ratio from the start of monotonic loading can be observed for assembly after dissipating the excess pore water pressure during liquefaction. Whereas the assembly without dissipating the excess pore water developed during liquefaction, shows a zero stress ratio up to an axial strain of 3% thereafter a sudden increase in the deviator stress with axial strain can be observed. However, beyond an axial strain of 3% both the assembly shows unique value of stress ratio.

![Graph showing stress ratio vs. axial strain](image3)

Fig.10: Variation of stress ratio with axial strain for assemblies with and without dissipating the excess pore water pressure developed during cyclic loading.

Variation of average coordination number with axial strain for samples with and without dissipating the excess pore water pressure during cyclic loading is presented in Fig. 11. The average coordination number increases gradually from 3.6 (at zero axial strain) and reaches a constant value of 4 at large strain levels for assembly after dissipating the excess pore water pressure during liquefaction. However, average coordination number increases from zero (point of liquefaction) to a value of 3, at an axial strain of 3% and further steadily increases to a constant value of 4 at large strain levels. It is interesting note that both the assemblies reaches a constant value of average coordination number at large axial strain (say $\varepsilon > 9\%$).

![Graph showing average coordination number vs. axial strain](image4)

Fig.11: Variation of average coordination with axial strain for assemblies with and without dissipating the excess pore water pressure developed during cyclic loading.

Dynamic Properties of granular materials

Shear modulus ($G$) and Damping ratio ($D$) are the two most important parameters for the dynamic analysis of granular materials. A typical hysteresis loop developed during cyclic triaxial loading is shown in Fig. 12. The slope of the secant line connecting the extreme point on the hysteresis loop is the Young’s modulus, $E$. The shear strain ($\gamma$) and shear modulus ($G$) can be computed from the following equations.
Where, $\mu$ = Poisson’s ratio and it is 0.5 for saturated undrained specimens. $\sigma_{d(max)}$ = maximum deviator stress; $\varepsilon_{max}$ = maximum axial strain.

Damping ratio, $(D)$ is a measure of energy dissipated to the maximum elastic strain energy and can be computed from the equation (7):

$$D = \frac{A_L}{4\pi A_T}$$  \hspace{1cm} (7)

Where, $A_L$ = area enclosed by the hysteresis loop, $A_T$ = area enclosed by the shaded triangle (see Fig.12).

Figure 13a,b,c presents the variation of shear modulus, peak compressional deviator stress ($q_{\text{max}}$) and the corresponding evolution of deviatoric anisotropic coefficient with shear strain. It is evident from the Fig. 13 that deviatoric anisotropy coefficient such as normal contact force anisotropy ($a_n^p$), fabric anisotropy ($a_f^p$) and tangential contact force anisotropy ($a_t^p$) remain constant at very low amplitudes of shear strain ($\gamma < 0.0025\%$). The assembly exhibit high values of average coordination number and shear modulus ($G$) (Fig. 6a). Since, there is no development of deviatoric anisotropy coefficients and displays higher value of $Z$, the assembly is said to be in Isotropic Zone ($IZ$). It is to be noted that $G$ exhibit higher value and remains constant in this zone.

In the Anisotropic Zone ($AZ$), $0.0025\% < \gamma < 1.00\%$, $q_{\text{max}}$ and $a_n^p, a_f^p, a_t^p$ steadily increases. In this zone, a continuous rearrangement and reorientation of particles takes place which results in the development of anisotropic coefficients. Moreover, there will be a net loss of contacts in the minor principal stress direction. As a result, $G$ and $Z$ drastically decrease in this zone. In Stable Anisotropic Zone ($SAZ$) ( $\gamma > 1.0 \%$) $q_{\text{max}}$ and $a_n^p, a_f^p, a_t^p$ and $Z$ remains constant. Consequently, $G$ also remains constant with a low value. This clearly highlight that anisotropic coefficient has a significant influence on the dynamic properties of granular materials.

Figure 14 presents the variation of modulus ratio ($G/G_0$) curve (value of $G_0$ corresponding to a shear strain of $10^{-3}\%$) with shear strain ($\gamma$) for the wide range of parameters such as confining pressure, void ratio, gradation, initial anisotropy, stress path considered for the study. Also presented in this figure, the lower and upper bound of modulus ratio curve as proposed by Seed and Idriss [34] and Kukusho and Esashi [35] for comparison. It can be observed that the numerical simulation results, irrespective confining pressure, void ratio, gradation, and stress paths are almost in the bounds as proposed by Seed and Idriss (1970) for clean sands. However, $G/G_0$ values for anisotropically compressed assembly falls below the lower bound curves of Seed and Idriss [34].

Figure 15 presents the combined plot of damping ratio ($D$) curve versus shear strain ($\gamma$) for the range of parameters considered for the study. Also presented in this figure, the lower and upper bound curves as proposed by Seed and Idriss [34] and Kukusho and Esashi [35] for comparison. It can be observed that the DEM simulation results irrespective confining pressure, void ratio, gradation, initial anisotropy.
and stress paths fall very close to the lower bound curves as proposed by Seed and Idriss [34] for clean sands. From these numerical simulation results it is very clear that DEM has captured realistically the influence of different parameters on the dynamic properties of granular materials.

Qualitatively captured all the features of the post liquefaction results. Moreover, numerical simulations using DEM have captured the variation of shear modulus and damping ratio with shear strain very similar to the laboratory experiments. The variation of shear modulus with shear strain can be divided into three zones (i) Isotropic Zone (IZ) (ii) Anisotropic Zone (AZ) and (iii) Stable Anisotropic Zone (SAZ). Comparison of DEM results with the experimental finding of past researchers showed that the normalized shear modulus ratio values for anisotropically compressed assembly fall below the lower bound of Seed and Idriss [34]. Whereas, damping ratio values lies close to the lower bound as proposed by Seed and Idriss [34].

Fig. 14: Relationship between modulus ratio with shear strain for different parameters considered for the present investigation [20].

Fig. 15: Relationship between damping ratio with shear strain for different parameters considered for the present investigation [20].

CONCLUSIONS

DEM simulations have captured the realistic behaviour of undrained cyclic response of granular media and have simulated the liquefaction, post liquefaction and dynamic properties of granular media similar to laboratory experiments. DEM results are comparable to the experimental results available in literature and it has captured the effect of different parameters very well. Liquefaction potential and pore water pressure generation exhibit an unique relationship irrespective of confining pressure, initial void ratio and amplitude of axial strains. The comparison of numerical simulation results with experimental findings of Dobry [33] indicates that there is a good agreement between the results of numerical simulation and the experimental results. Moreover, numerical simulations using DEM have qualitatively captured all the features of the post liquefaction undrained behaviour of granular materials very similar to experiments. Amplitude of axial strain required for initial liquefaction has a significant influence on the post liquefaction undrained stress strain response. Moreover, the DEM numerical results have captured the variation of shear modulus and damping ratio with shear strain very similar to the laboratory experiments. The variation of shear modulus with shear strain can be divided into three zones (i) Isotropic Zone (IZ) (ii) Anisotropic Zone (AZ) and (iii) Stable Anisotropic Zone (SAZ). Comparison of DEM results with the experimental finding of past researchers showed that the normalized shear modulus ratio values for anisotropically compressed assembly fall below the lower bound of Seed and Idriss [34]. Whereas, damping ratio values lies close to the lower bound as proposed by Seed and Idriss [34].

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