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Abstract

Methane gas hydrates are crystalline compounds formed from water and methane under certain pressure and temperature. They are mostly found in marine continental margin sediments and beneath the permafrost and considered as the future non-conventional energy resource. In order to develop innovative techniques for the safe extraction of methane gas from Methane Hydrate (MH) it is important to understand the shear behaviour of methane hydrate bearing sand. It has been reported that the pore scale habits of MH have a significant influence on the shear behaviour of methane hydrate bearing sand. In this paper, an attempt has been made to capture the effect of pore scale habits on the shear behaviour of methane hydrate bearing sand using the Discrete Element Method. Two modelling approaches (i) pore filling, leading to load bearing, and (ii) cementation, bonding of the interparticle contact, have been simulated using PFC3D. A series of triaxial monotonic tests were carried on an assembly of particles for different methane hydrate saturations. Both the approaches have captured, qualitatively, the stress ratio-axial strain behaviour similar to the laboratory experiments. The DEM simulation results highlight that MH saturation has a profound influence on the shear behaviour of hydrate bearing sand. It was shown that the cementation habit closely captures the variation of peak deviator stress with MH saturation similar to the laboratory experiments. Moreover, the evolution of micro-mechanical parameter (e.g. contact force and bond breakage) during shear loading has been presented and discussed.

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DEM MODELING OF METHANE HYDRATE BEARING SAND

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ABSTRACT

Methane gas hydrates are crystalline compounds formed from water and methane under certain pressure and temperature. It is mostly found in marine continental margin sediments and beneath the permafrost and considered as the future non-conventional energy resource. In order to develop innovative techniques for the safe extraction of methane gas from Methane Hydrate (MH) it is important to understand the shear behaviour of methane hydrate bearing sand. It has been reported that the pore scale habits of MH have a significant influence on the shear behaviour of methane hydrate bearing sand. In this paper, an attempt has been made to capture the effect of pore scale habits on the shear behaviour of methane hydrate bearing sand using the Discrete Element Method. Two modeling approaches (i) pore filling, leading to load bearing, and (ii) cementation, bonding of the interparticle contact, have been simulated using PFC3D. A series of triaxial monotonic tests were carried on an assembly of particles for different methane hydrate saturations. Both the approaches have captured, qualitatively, the stress ratio-axial strain behaviour similar to the laboratory experiments. The DEM simulation results highlight that MH saturation has a profound influence on the shear behaviour of hydrate bearing sand. It was shown that the cementation habit closely captures the variation of peak deviator stress with MH saturation similar to the laboratory experiments. Moreover, the evolution of micro-mechanical parameter (e.g. contact force & bond breakage) during shear loading has been presented and discussed.

1 INTRODUCTION

In Australia, three-quarters of energy comes from coal, 14 percent from natural gas, 8 percent from renewable sources (mainly hydroelectric, wind power and bioenergy) and 1 percent from oil according to ANSTO. However, natural gas is the cleanest of all the fossil fuels, emitting from 25 - 50 percent less carbon dioxide than either oil or coals for each unit of energy produced. Recently, offshore geologic survey has shown that the oceans and polar terrestrial masses around the world hold immense amounts of methane (the primary component of natural gas) concentrated in cage-like ice structures known as methane hydrates. The methane hydrates are considered as one of the most feasible sources for energy compared with other known hydrocarbon deposits for future. However, there is significant hazard during drilling and production operations for methane hydrate as the methane is approximately 20 times as effective as green house gas as carbondioxide (e.g. Hyodo et al. 2005; Collet & Dallomore, 2002) and highly unstable. To produce methane gas from methane hydrate safely and without damaging the environment, we need to address a wide-range of geotechnical and environmental issues. For instance, it has been reported that methane hydrate production may collapse and leads to settlement or landslides on the seabed. Moreover, marine substructures are vulnerable to the sea bed deformations and no attractive technology is currently available to recover methane economically from methane hydrate. Till date, large scale production has not yet commenced as the behaviour of gas hydrates, particularly hydrates of methane, are not fully understood. However, a lot of research on MH as a future energy source has been reported, recently, which shows that countries are eager to develop an effective way to capture MH in order to secure their natural gas stores for the future and also an attempt to combat global warming (e.g. Kvenvolden, 1988; Waite et al., 2009; Collet, 2002; Kvenvolden and Lorenson, 2001; Hyodo et al., 2013).

Recently, the laboratory experiments such as triaxial, direct shear and bending tests have been conducted on the shear behaviour of methane hydrate bearing sediment (e.g. Masui et al 2005; Hyodo et al 2002, 2005 & 2013 and Song, 2010). Experimental results highlight that the shear strength, stiffness and dilation of hydrate bearing sand is influenced by hydrate saturation, initial confining pressure and temperature. Waite et al. (2009) concluded that stress- strain response of hydrate bearing soil is affected by the hydrate growth habit. They have described three models which show the microscopic distribution of hydrates in soils. (1) pore filling: hydrate nucleate on sediments grain boundaries and grow freely into pore spaces without bridging two or more particles. (2) load-bearing: Hydrate bridges neighboring grains and contributes mechanical stability to granular assembly by becoming part of the loading bearing force chain. (3) Cementation: Hydrate establish a bond on the interparticle contact points. While the different habits of MH within the host sediments are generally accepted, the specific pore-scale interactions between coarse grained sediments and MH molecules are less understood. Jung et al (2012) reported that it is highly difficult to control hydrate formation, distribution, saturation, and pore habit challenges during laboratory experiments. In this context, numerical simulations

using DEM will provide valuable insight on the hydrate formation and the micromechanical interaction between sand-sediment mixtures. This is mainly because the DEM is structured from the modeling of the particles at the grain scale level. The advantage of this method is that it has the flexibility in facilitating the isolation effects, the loading configurations and individual particle characteristics such as size, shape, roughness and physical properties in relation to the mechanical behaviour of the assembly. Brugada et al (2010) developed a DEM model to capture shear behaviour of methane hydrate soil considering the pore filling distribution. It has been highlighted that hydrate contribution to the strength of the sediment is purely frictional nature. Jung et al (2012) carried out DEM simulations to explore the effects of hydrate distribution, saturation, sediment porosity, confining stress and pore habit. They concluded that mechanical properties of hydrate-bearing sediments can be expressed as function of hydrate saturation, initial porosity and effective stress. Jian et al (2013) developed a simple contact model to capture the cementing effect of methane hydrate sediment mixtures. They reported that the cohesion/cementation of hydrate bearing deposit increases with increase in hydrate saturation. Vinod et al (2014) investigated the pore filling distribution and shown that MH particles strongly contribute towards load bearing arrangement and hence exhibit an increase in deviator stress with MH. In this study, pore filling habit, load bearing, and cementation habit, bonding on the interparticle contact point, has been investigated using DEM simulations. The effect of hydrate saturation and micromechanical interaction between sand and MH has been studied and reported.

2 DISCRETE ELEMENT METHOD

The Discrete Element Method (DEM) also known as the distinct element method, was originally proposed by Cundall and Strack (1979) for dry granular particles. DEM models simulate the movement and interactions of spherical particles and determine the equilibrium contact forces, stresses and displacements of the individual particles. The calculation process (Fig.1) for the DEM involves alternation between the application of Newton's second law of motion and the force-displacement law (Itasca, 2004). Newton's second law of motion is solved using the explicit finite difference procedure, which determines the motion of each particle arising from its contact forces. The force displacement law is then used to update the contact forces arising from the relative motion at each contact (Itasca, 2004). DEM software (PFC3D) treats individual particles as an assembly of discrete elements that makes up a solid area or volume of material, which is bound by walls. The particles are assumed to be spherical, rigid and of negligible contact area (that is, contact at only a point), but are allowed to overlap at contacts via the soft contact approach, determined through the force-displacement law (Itasca, 2004). PFC3D enables the investigation of features that are not easily measured in laboratory tests such as co-ordination numbers, inter-particle contact forces, and the distribution of normal contact vectors and it is also possible to compose bonded particles using contact bonding or parallel bonding into agglomerates and simulate fracture when the bonds break. A parallel bond can be idealised as a set of elastic springs with a constant normal and shear stiffness, uniformly distributed over a circular disk lying on the contact plane and centred at the contact point between two balls (Itasca, 2004). It is this circular or cylindrical disk that represents the cementation between two particles (See Fig 2). Parallel bond can be described by the following five parameters: normal and shear stiffness, normal and shear strength and bond disk radius (R).

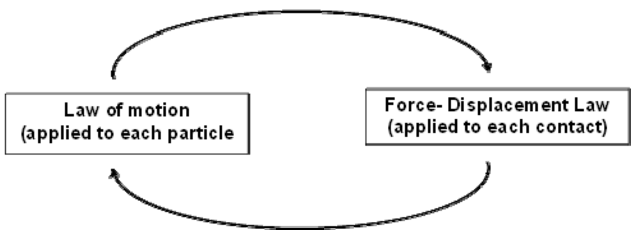

Fig.1: Calculation cycle used in PFC3D (Itasca, 2004)

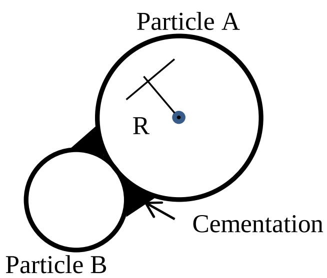

Fig.2: Parallel bond logic used in PFC3D (Itasca, 2004)

The maximum tensile and shear stresses acting on the periphery of the bond (Itasca, 2004) are given by:

$$\sigma_{\max} = \frac{-\bar{F}^n}{A'} + \frac{\left|\bar{M}_i^s\right|}{I}\bar{R} \qquad (1)$$

$$\tau_{\max} = \frac{\left|\bar{F}^s\right|}{A'} + \frac{\left|\bar{M}^n\right|}{J}\bar{R} \qquad (2)$$

where $\sigma_{\max}$ and $\tau_{\max}$ are the maximum tensile and shear stresses acting on the periphery of the bond, $\bar{F}^n$ and $\bar{F}^s$ are the normal and shear forces acting on the bond, $\bar{M}_i^s$ $\bar{M}^n$ are the normal and shear moment acting on the bond, R is the radius of the bond, and A', I and J are the area, moment of inertia and polar moment of inertia respectively of the cross section of the bond.

3 LABORATORY EXPERIMENT ON MH BEARING SAND

Recently, a series of triaxial laboratory experiments were carried out by Hyodo et al. (2005 & 2013) on the methane hydrate bearing sand samples. Toyoura sand was selected as the MH bearing sand (host sand). The cylindrical specimen of 30mm diameter and 50 mm high were prepared at an initial porosity of 0.4. To simulate the pressure and temperature conditions favorable for MH formation and stability, a rigorous preparation procedure was developed and followed by Hyodo et al. (2013). MH bearing sand was first mixed with predetermined amount of water to achieve the target MH saturation. The moist soil was then placed in a mold with each layer compacted by tamper. This specimen was then subjected to a series of process under specific temperature and pressures as shown in Fig. 3. The methane gas was injected at stage (3) and the temperature was reduced to 1C where MH was stable (Fig.3). A very high pore water pressures was then applied to the sample to consider the condition of the sea bed. More details on the sample preparation and testing procedure can be found elsewhere (e.g. Hyodo et al 2013 & 2005). Drained triaxial tests were carried out on MH bearing sand with varying MH saturations.

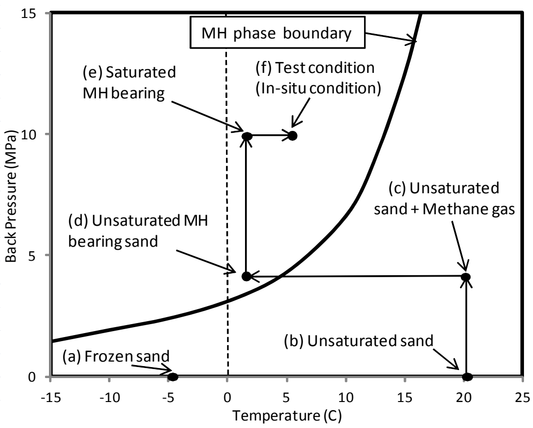

Fig. 3: State paths for pressure and temperature to produce MH bearing sand (after Hyodo et al., 2013)

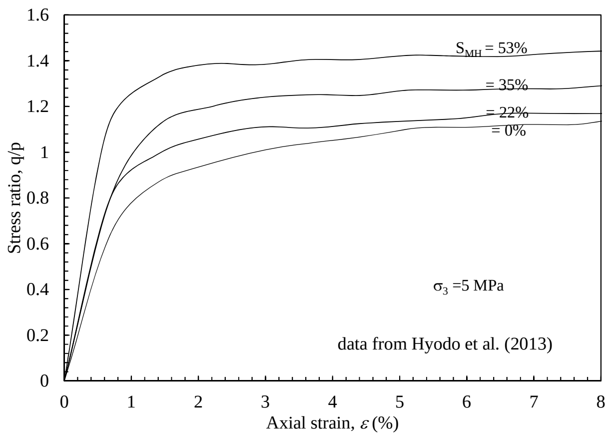

Fig.4: Effect of MH on the stress ratio with axial strain for MH bearing sand (after Vinod et al 2014)

Fig. 4 shows the variation of stress ratio and volumetric strain with axial strains for samples with different percentage of MH saturation. It is shown that MH saturation has profound influence on the shear behaviour of MH bearing sand. A significant increase in the initial stiffness and shear strength was observed with increase in the MH saturation. The increase in shear strength with MH saturation may be due to the cementation/bonding of sand particles of sandy sediments beneath the deep ocean floor (Hyodo et al. 2013).

4 DEM SIMULATIONS OF MH BEARING SAND

DEM simulation very similar to the laboratory experiments were carried using PFC3D. The cylindrical soil specimen (diameter =30mm, height = 60mm), similar to the size of the laboratory experiments, was prepared from 7941 spherical

particles. The particle size varying from 0.07 - 1 mm was considered for MH bearing sand (host sand). The MH bearing sand samples were prepared at an initial porosity of 0.4. During sample preparation the particles were randomly located inside the container without any overlap with the existing particles. The cylindrical lateral wall was assigned a stiffness of 5E7 N/m to create a soft confinement. The particles were generated using radius expansion technique incorporated in PFC3D. After generation the assembly was isotropically compacted to a desired initial confining pressure (σ). The properties used for MH bearing sand are tabulated in Table 1. A linear force displacement contact model was used for the simulation program.

4.1 MODELLING OF PORE FILLING HABIT: The MH particles were randomly generated in the pores of the sand particles as described in the earlier section. The number of particles for different saturation was determined from initial void volume. The MH particles were assumed to be of uniform spherical particles having a size 0.04 mm. The random process was repeated until the total number of specified hydrates was created to reach desired hydrate saturation. The properties assigned for the MH particles are presented in Table 1. It was observed that the initial porosity slightly decreases with the addition of MH particles. The samples with different hydrate saturation are presented in Fig. 5. A series of drained monotonic triaxial tests were then carried out by applying a constant velocity of $1x10^{-5}$ m/s at the top and bottom platen.

Table 1: Micromechanical Properties used for DEM simulations (after Vinod et al. 2014)

Properties	Soil	Methane Hydrate
Density (kg/m^3)	2000	2000
Normal Stiffness (N/m)	5E8	1E9
Shear Stiffness (N/m)	5E8	1E9
Particle Size (mm)	0.07-0.1	0.04
Contact friction	0.52	0.58 (S_{MH} = 22%); 0.61 (S_{MH} = 35%); 0.64 (S_{MH} = 53%)

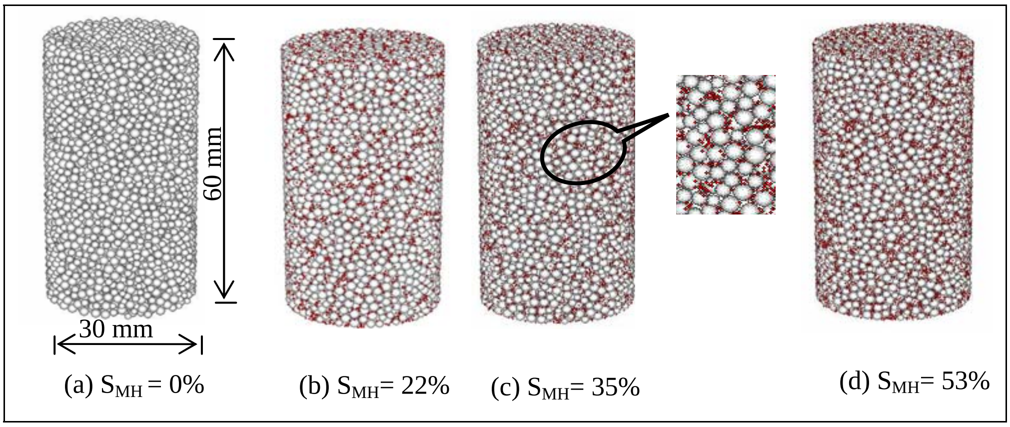

Fig.5: Initial assembly with different percentage of MH (after Vinod et al. 2014)

4.2 MODELLING OF CEMENTATION HABIT: The cementation effect of MH was introduced using a parallel bonding model. Parallel bond approximates the physical behaviour of a cement-like substance joining two particles. It can transmit both forces and moments between particles, thus, they may contribute to the resultant force and moment acting on the two bonded particles (Itasca, 2004). It has been reported that bond strength (cementation) of the methane hydrate bearing sand increases with increase in MH (Hyodo et al. 2009 and Jiang et al., 2013, 2014). Therefore in this study, the bond strength of the assembly has been varied to capture the shear behaviour for different percentage of MH saturation (see Table 2). A bond shear and normal stiffness of 1E9 N/m and bond radius of 0.2-0.6 m was used for the simulations. A series of drained monotonic tests were carried out on the initial sample (Fig.5a) varying the normal and shear bond strength to capture the effect of MH saturation.

Table 2: Micromechanical properties used for DEM simulations

MH Saturation (%)	Normal & Shear Bond Strength (N/m^2)
0	0
22	8.0E6
35	1.2E7
53	1.5E7

5 RESULTS AND DISCUSSIONS

5.1 PORE-FILLING HABIT

Fig. 6 shows the variation of stress ratio with axial strain for different percentages of MH saturation at an initial confining pressure of 5 MPa. It is clear from the figure that MH saturation has significant influence on the shear behaviour of sand. The stress ratio increases with the increase in the methane hydrate saturation. The stress ratio exhibit a peak value around 2% axial strain thereafter remains constant with axial strain. Qualitatively, this result is very similar to the laboratory experimental results presented by Hyodo et al. (2013). The variation of peak deviator stress with confining pressure for different MH saturation is presented in Fig, 7. It is shown that peak deviator stress increases linearly with confining pressure irrespective of MH saturation. As expected, peak deviator stress increases with MH saturation. Moreover, significant influence of MH saturation on the peak deviator stress can be observed for $\sigma_3 > 3$ MPa.

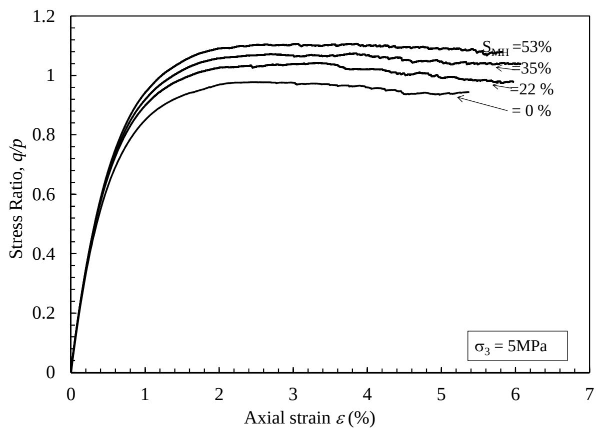

Fig.6: Effect of MH on the deviator stress and volumetric strain with axial strain for MH bearing sand (after Vinod et al. 2014)

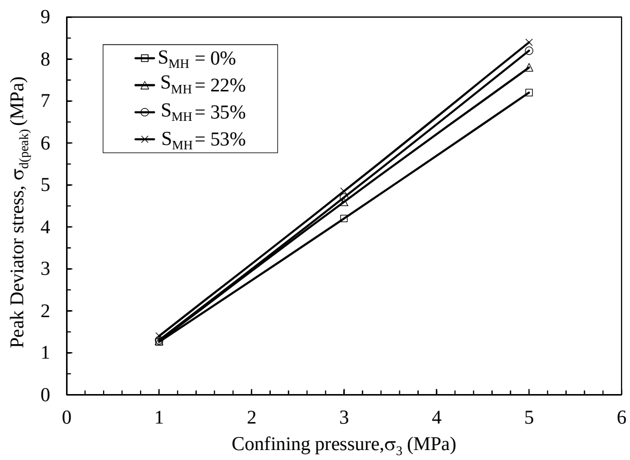

Fig.7: Variation of peak deviator stress with confining pressure for different MH saturation (after Vinod et al 2014)

The spatial variation of contact force (CF) chain developed during shear loading for samples S_{MH}= 0% and S_{MH}=35% is presented in Fig 8. Fig.8 (a) shows the CF developed for MH bearing sand (S_{MH}=0%) samples at ε = 0.35%. Whereas, Fig. 8(b) shows the CF distribution for S_{MH}=35% at ε = 0.35%. The contact force is represented by a line segment connecting the centriod of two contacting particles, and the line width is proportional to contact force magnitude. During shear loading CF chains are developed along the major principal stress direction. It is evident from Fig.8b that the MH particles strongly contribute to load bearing along with MH bearing sand during shear loading. It is evident that mean CF (the average value, overall contacts with non-zero normal force) increases with increase in the axial strain. The mean contact force of 0.9 MN and 1.1MN was observed for samples S_{MH}= 0 and S_{MH} = 35 % respectively at ε =1.0%. In fact, the increase of CF with MH saturation is directly reflected in the corresponding increase in deviator stress (Fig.7).

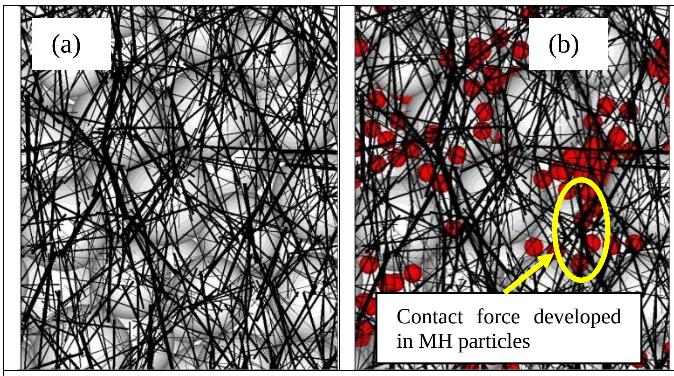

Fig.8: Spatial variation of contact force chain during shear loading (a) S_{MH} =0% ε = 0.35% (b) S_{MH} =35%; ε =0.35% (after Vinod et al. 2014)

5.2 CEMENTATION HABIT

Fig.9 shows the variation of stress ratio with axial strain for different percentage of MH. It is evident from the figure that that cementation habit has also captured the influence of MH saturation similar to the laboratory experiments. As anticipated, DEM simulation clearly shows that the peak strength increases with increase in the MH saturation.

The mechanism controlling the behaviour of the cemented MH bearing sand model is the breakage of the bonds. Fig.10 shows that the breaking of bonds has a significant influence on the shear behaviour of cemented MH bearing sand. In PFC3D, a parallel bond break if the magnitude of the tensile normal or shear contact force exceeds the applied normal or shear bond strength. This is clearly demonstrated in Fig. 10, where at low strains all bonds remain intact, however, during shearing CF increases and when CF exceeds the bond strength the bond breaks. The bond breaks non-linearly with axial stain and expected to reach a steady state at large strain (ε >10%). For a particular value of axial strain bond breakage decreases with increase in MH saturation, hence, exhibit higher shear strength.

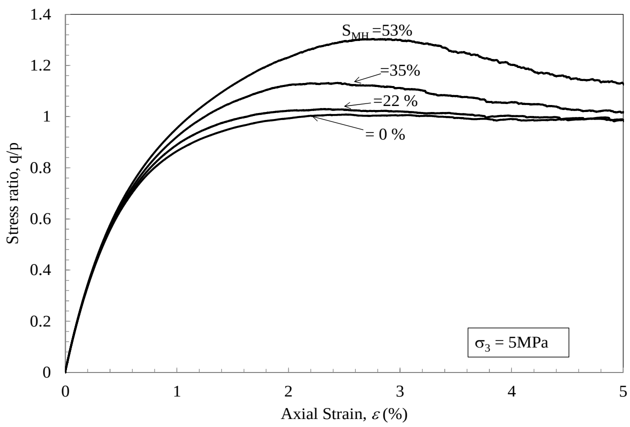

Fig.9: Effect of MH on the deviator stress with axial strain for MH bearing sand

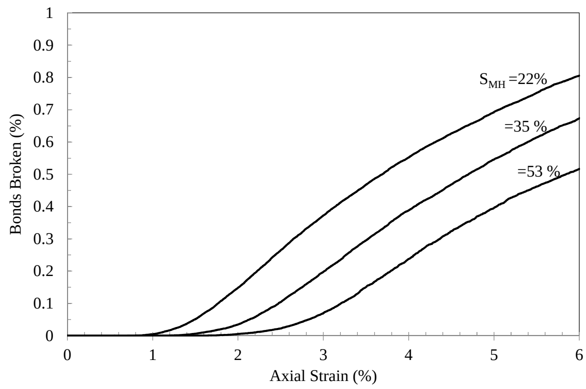

Fig.10: Variation of broken bond with axial strain for different MH saturation

Fig.11 a &b shows the spatial variation of parallel bond with axial strain. The parallel bond locations are shown by black line between two particles for the specimen with MH saturation of 35% at ε = 0% and ε= 5% . Fig. 11 (a) shows all the bonds (cementation) developed before shearing. During shear loading, CF develops and when this exceeds the bond strength, the bond breaks. Fig.11(b) clearly shows the development of CF leading to the breakage of bond (cementation). The bond breakage is expected to reach a steady state at large axial strain levels.

5.3 COMPARISON WITH LABORATORY EXPERIMENTS

Fig.12 shows the comparison of DEM simulations results with laboratory experiments carried out Hyodo et al (2013). It is evident from the figure that cementation habit clearly captures the variation of peak deviator stress close to the laboratory experiments. The pore filling habit shows a close agreement at low MH saturation (S_{MH} < 20%), however, did not capture the increase in deviator stress at high MH saturation (S_{MH}>20%). This result clearly demonstrates the development of a cementation type hydrate growth habit on the Toyoura sand during laboratory experiments.

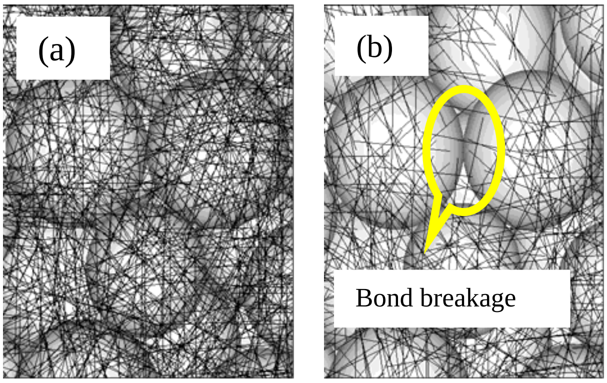

Fig.11 Spatial variation of parallel bond with axial strain (a) ε = 0%; (b) ε = 5%

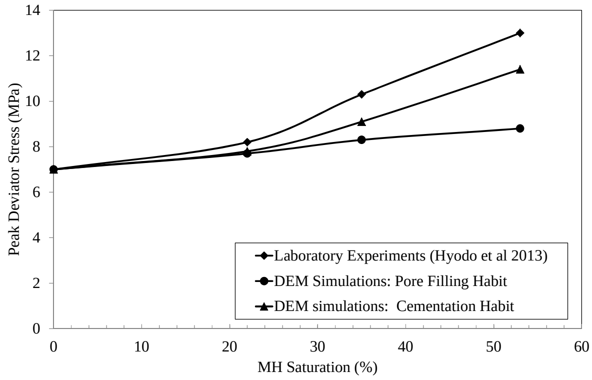

Fig.12. Comparison with Laboratory experiments

6 LIMITATIONS

The major aim of this study is to understand the pore scale habit on the shear behaviour of MH bearing sand. Although the DEM analysis albeit certain simplified assumptions could capture the shear behaviour of MH bearing sand to a significant extent, the future studies should overcome the following the limitations.

1. In this study, only stress- strain response of MH bearing sand was simulated; however, simulations should be extended to capture the volumetric strain behaviour for different MH saturation.
2. DEM model did not capture the increase in stiffness observed in the laboratory experiments. This may be due to the lack of information on the proper input (micromechanical) parameters, especially stiffness, for the simulation. Detailed laboratory experiments should be carried out on constant stiffness shear equipment to evaluate the most appropriate values of the normal and the shear stiffness for sand with and without cementation.
3. The effect of cementation of MH bearing sand was captured by varying the bond strength; this is mainly because of the lack of information on the bond strength with MH saturations. Laboratory experiments have to be carried out to establish a relationship between bond strength and MH saturation.

7 CONCLUSIONS

This paper has presented the results on the shear behaviour of MH bearing sand using DEM. Two distinct approaches, (i) pore filling and (ii) cementation habit were simulated to capture the stress-strain response of MH bearing sand. The shear behaviour of MH bearing sand for different MH saturation has been simulated by varying the contact friction angle for pore filling habit and bond strength for cementation habit respectively. It was shown that both the approaches have qualitatively captured the stress ratio – axial strain variation similar to the laboratory experiments. It can be concluded from DEM simulations that the stress ratio significantly increases with increase in MH saturation. Moreover, DEM simulations highlights that the cementation type hydrate growth may exist during shear loading of Toyuora sand in laboratory condition. The DEM based micromechanical analysis shows that in pore filling habit MH particles strongly contribute towards the overall load bearing arrangement and in cementation habit the breakage of bond (cementation) decreases with the increase in MH saturation.

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