DEM analyses of cemented hydrate’s effect on the compression behavior of fine-grained sediments

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Abstract. The participation of gas hydrate constitutionally affects the mechanical properties of gas hydrate-bearing sediments. The hydrates contribute to the mechanical properties of hydrate-bearing sediments by pore-filling, bearing and bonding effects. A discrete element model of hydrate-bearing silt was established randomly filled by the hydrate particles into silt-sized granular skeleton reservoir. The cluster & bonding hydrate is generated in the pores of the numerical silt reservoir to study hydrate’s mechanical effects. One-dimensional loading was applied to the numerical sample to investigate its volume change, bond degradation and stress transmission. The main conclusions are as follows. The structural yield stress corresponds with the abrupt bond breakage. Particles and contacts will be redistributed after the widespread bond breakage. The breakage of hydrate-hydrate bonded contacts is more quickly than that of silt-hydrate contacts ascribe to a crushing process of hydrate clusters (especially for $S_{MH}=45\%$).

1. Introduction

Methane hydrates form in the pore space of the permafrost and continental margin sediments at high pressure and low temperature conditions. The microstructural growth of hydrate within the interior of pores controls the mechanical properties of the sediment [1]. Hydrate particles randomly grow in the pores of granular skeletons, which densifies the sediment. With the increasing of hydrate saturation (hydrate volume to pore volume ratio), hydrate bridges neighboring graduates and contributes to the mechanical stability of the granular skeleton, which is pore-filling and bearing effects. In some sediments, the inter-granular hydrate cements the skeleton grains together and evidently change the properties of the sediments, which is bonding effect. In practice, pore-filling, bearing and bonding effects could coexist.

The microstructures of hydrate-bearing sediments can be achieved by microcosmic observations while micromechanical properties could not, such as bonding degradation and stress transmission through contacts. The discrete element method (DEM) [2] has been regarded as an alternative and effective tool to correlate the macro- and micromechanical behavior of granular materials. Hydrate-bearing sands that reproduce the primary macroscopic mechanical properties of sands with particulate pore-filling hydrates [3], clump pore-filling hydrates [4] or virtual bonding hydrates [5] have been analyzed and simulated by the DEM. However, few investigations focus on the overall effect of pore-filling, bearing and bonding effects.
The accumulation of methane hydrates in fine-grained sediments exceeds the accumulation in sands. However, hydrate-bearing fine-grained sediments remain less understood and characterized than sandy reservoirs. This paper aims to analyze the effect of hydrates on the mechanical behavior of fine-grained granular sediments by using the DEM. Hydrate-bearing silts were produced by using the PFC code; the hydrate particles are cemented together to reproduce the pore-filling and bearing effects of hydrate clusters and the hydrate particles are cemented to the silt skeleton particles to reproduce the bonding effect. A series of one-dimensional compression tests were numerically performed on the DEM samples to investigate the macroscopically mechanical behaviors of the hydrate-bearing silt and its micro-mechanism such as bond degradation and stress transmission through contacts.

2. DEM simulation

2.1. Contact model and parameters

In the applied contact model, interparticle rolling and twisting resistances [6] were incorporated to consider the particle shape effect and particle surface roughness in sphere-based DEM simulations; interparticle van der Waals force were taken into account to simulate silt-sized soils [7]; and cementation bond were installed to consider the bonding effect of hydrates [8].

The contact force and moment at a contact between bonded particles are assumed to be transmitted by particle interaction and cementation bond, which gives \( F = F^p + F^b \) and \( M = M^p + M^b \), where, \( F \) and \( M \) are the contact force and moment, \( F^p \) and \( M^p \) are the force and moment transmitted by particle interaction, and \( F^b \) and \( M^b \) are the force and moment transmitted by cementation bond. The calculation of \( F^p, M^p, F^b \) and \( M^b \) and the microscopic parameters please refer to Li et al.[7] for detail. The interaction parameters on silt-silt, hydrate-hydrate and silt-hydrate contacts and cementation bond parameters on hydrate-hydrate and silt-hydrate contacts are listed in Table 1.

| Parameter | Value | Parameter | Value |
|-----------|-------|-----------|-------|
| Effective modulus \( E^*/\text{MPa} \) | 800/80 | Bond effective modulus \( E^*/\text{MPa} \) | 20 |
| Normal-to-shear stiffness ratio \( \kappa^* \) | 1.5/1.5 | Bond-to-particle modulus ratio \( \eta_E \) | 1 |
| Friction coefficient \( \mu \) | 0.5/0.04 | Bond normal-to-shear stiffness ratio \( \kappa^* \) | 2.0 |
| Contact radius multiplier \( \beta \) | 0.1/0 | Bond compressive strength \( \sigma_c^b/\text{MPa} \) | 5 |
| Local crushing parameter \( \zeta \) | 2.1/0 | Tension-to-compression strength ratio \( \eta_{\sigma} \) | 0.1 |
| Bond radius multiplier \( \lambda_b \) | | Bond thickness threshold \( g_c \) | 0.8 |

2.2. Sample modeling and DEM execution

Silty particles were selected based on the representative grain size distribution and median particle diameter from hydrate explorations of Shenhu Area, Northern South China Sea. Hydrate particles were filled in the pores of soil skeletons. The specific diameter of hydrate particles \( d_{MH} \) was given with a fixed value of 9 \( \mu \)m. The value of hydrate saturation \( S_{MH} \) (hydrate volume to pore volume ratio) was 0%, 10%, 25%, 35% and 45% respectively. Figure 1 shows the grain size distribution curve of the DEM samples. The particle density of silt was 2710 kg/m\(^3\), while hydrate particles was 900 kg/m\(^3\). Local damping was adopted with a coefficient value of 0.7.
The numerical samples were prepared as follows. (1) Silty skeleton production. A cubic assembly composed of 7823 particles with a side length of 0.2 mm and a target void ratio of 1.08 was prepared firstly. (2) Hydrate filling. Hydrate particles were filled inside the soil skeletons randomly after that, with each of their six boundaries under a fixed boundary condition. (3) Precompression. A vertical pressure of 10 kPa was applied to the samples with the side walls fixed to reproduce an in-situ $K_0$ stress state. (4) Bond installation. After precompression, cementation bonds were installed at hydrate-hydrate and silt-hydrate contacts with a gap less than $g_cR_b$. The DEM sample with $S_{MH}=25\%$ after sampling are shown in Figure 2.

A van der Waals force was applied to each ball-ball contact because it cannot be neglected in sample preparation for a silt-sized assembly [9]. When particle surfaces are in contact across their interface, van der Waals force could be calculated with Eq.(1) as follows [10]:

$$F_v = \frac{H_a R_b^2}{6h^3}$$

where $H_a=6.5 \times 10^{-20}J$ is the Hamaker constant, $h=2$ nm is the separation of surfaces along the line of the centers of adjacent particles. The value of $R_0$ was equal to $R_c$ when particle surfaces were in unbonded contact, while $R_b$ in bonded contact.

During one-dimensional compression, continuous vertical loads were applied by moving the top and bottom walls downward and upward respectively, with the side walls keeping stationary.

3. DEM simulation results

Figure 3 shows the variation in void ratio. The calculation method of void ratio in this research considers both hydrate particles and silty particles as solid particles. The compression curve presents a distinct structural yield stress. Samples with a lower hydrate saturation value has a more apparent structural yield phenomenon compared with a higher hydrate saturation; hence, bonding effect has significant influence on compression properties in regard to samples with large void ratio.

The bond breakage of different contact types of granular assembly is a key scientific problem. There are three contact types in the samples, including silt-silt contact (C_s-s), hydrate-hydrate contact (C_h-h), and silt-hydrate contact (C_s-h). There are cementation bonds at silt-hydrate contact and hydrate-hydrate contact.

Figure 4 presents the process of bond breakage in the samples. There are barely bond breakages until it reaches the inflection point (bond crushing stress) with the applying of mean stress $p$. Once the inflection point is reached, the bonds would break rapidly. Moreover, the growth inflection point is related with the structural yield stress. If the sample has a significant structural yield stress, the moment the structural yield stress reaches, the moment the bond would break rapidly, such as sample with $S_{MH}=10\%$; as to those samples have no significant structural yield stresses, the inflection point could be assisting in finding its structural yield stress, for example, sample with $S_{MH}=45\%$.

When $S_{MH} \leq 35\%$, the initial bonded number of C_s-h is more than C_h-h. When $S_{MH}=45\%$, the initial bonded number of C_s-h is less than C_h-h, because of more hydrate fillings; the breakage of bonded C_h-h is
slightly earlier and much more quickly than that of bonded C_s-h, which shows a crushing process of hydrate clusters.

The stress of a granular assembly are dependent on the interparticle interaction at contacts. The average stress of a representative volume element can be expressed as follows [11]:

$$\sigma_{ij} = \left( \sum_{k=1}^{C} F_{ik} l_{jk} \right) / V$$

where $V$ and $C$ are the volume and the number of contacts of the assembly, respectively; $F_{ik}$ is the contact force at contact $k$ and $l_{jk}$ is the branch vector connecting the centers of the two particles.

The mean stress transmitted by different contact types can be calculated by the average stress tensor. Figure 5 illustrates the mean stresses transmitted by C_s-s, C_h-h and C_s-h, respectively. Solid lines describe the compression curves, while dash, dot and dash-dot present the mean stresses transmitted by C_s-s, C_h-h and C_s-h respectively, which are $p_{s-s}$, $p_{h-h}$ and $p_{s-h}$, and the sum of those three stresses equals $p_{s-h} + p_{s-h}$. Could be described as the mean stress transmitted by hydrate particles, which is presented as the difference of solid and dash lines on the abscissa axis.

The compression curves have significantly structural yield stress, $p_{h-h}$ and $p_{s-h}$ also have inflection point when the compression curves reach their yield stress. Take $S_{MH}=25\%$ as an example, there are relatively large difference between solid and dash lines near the structural yield stress, which means hydrate stands large magnitude of the total stress near the structural yield stress. However, when it goes to a lower mean stress, hydrate bond hardly has any significant effect; simultaneously, after the widespread bond breakage, hydrate also contributes to a smaller proportion of the total stress.
4. Conclusions
This paper simulates cemented hydrate-bearing fine-grained sediments by using a DEM code. A series of one-dimensional compression tests were numerically performed to investigate the macroscopical mechanical behaviors of the hydrate-bearing silt and its micro-mechanism such as bond degradation and stress transmission. The main conclusions are as follows:

1. Based on compression curves of the DEM simulations, there is structural yield stress associated with widespread bond breakage. If the sample has a significant structural yield stress, the moment the structural yield stress reaches, the moment the bonds break rapidly (\(S_{MH}=10\%\)); as to those samples with no significant structural yield stress, the inflection point could assist in finding its structural yield stress during simulation carried on.

2. The stress inflection point of the breakage of bonded \(C_{b,h}\) is slightly lower than that of bonded \(C_{s,h}\) when bonds break, and the bond breakage of \(C_{b,h}\) is much more quickly than that of \(C_{s,h}\), which shows a crushing process of hydrate clusters, especially for the sample with \(S_{MH}=45\%\).

3. Silty skeleton shares an increasing proportion of mean stress with the applying of pressure. Because of the cementation bonds, the most proportion of the mean stress shared by hydrate is near the structural yield stress.

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