Discrete element modeling of the effect of particle size distribution on direct shear behavior of hydrate-bearing sediments

Anna Qian¹, Yanlu Ding², Hailong Lu¹-²

¹ School of Earth and Space Sciences, Peking University, Beijing, China
² Beijing International Center for Gas Hydrate, Peking University, Beijing, China

Abstract. Natural gas hydrates are a new energy resource with a great potential for commercial exploitation. The exploitation of natural gas hydrate can cause a degradation of the mechanical properties of hydrate-bearing sediments (HBS) and may trigger geohazards. Natural gas hydrates exist widely in marine sediments which have different types of sediment matrix with different particle size distributions (PSD). The effect of the PSD of hydrate-bearing sediments has not been investigated clearly. In this paper, a direct shear test model of HBS is built using the discrete element method. A series of numerical simulations with different PSD of HBS under different hydrate saturations and vertical stresses are conducted. The results show that the shear strength, residual strength, and dilatation of HBS increase with increasing hydrate saturation at the same PSD. It is found that the mechanical properties of HBS are not sensitive to the PSD at the same median particle size at low vertical stress. However, the shear strength can be enhanced with the increase of median particle size. The results obtained in this study can facilitate a deep understanding of the mechanical properties of HBS.

1. Introduction
Natural gas hydrates are ice-like compounds and are composed of water and gas molecules. They are usually formed in deep marine sediments and permafrost regions where provide high pressure and low-temperature environment [1, 2]. They are considered a clean energy resource compared to traditional fossil fuels. They have been identified as a great potential for commercial exploitation [1, 3]. The extraction of natural gas hydrates can cause a degradation of the mechanical properties of hydrate-bearing sediments (HBS) and induces geohazards, which may impede the long-term safe commercial exploitation of gas hydrate. Therefore, it is important to understand the mechanical properties of HBS [4]. The marine sediments that natural gas hydrates occurred in have a wide range of different particle size distributions (PSD). Previous studies have demonstrated the PSD of sediment matrix can influence the mechanical properties of HBS. Miyazaki et al. [5] conducted drained triaxial compression tests on artificial HBS formed with different hosting sands of different average particle sizes. They also found the stiffness of HBS depends on the type of sand, while the strength has little dependence on the type of sand. Waite et al. [6] obtained that the PSD can influence the saturation and distribution of the gas hydrates according to the field studies. Hyodo et al. [7-8] performed a series of triaxial tests to study the mechanical properties of HBS with different fines contents. The result indicates that the particle size of the sediment matrix can affect particle bonding. With the increase in fines content, the void ratios of hosting sediments tend to decrease and the hosting sediments become denser, leading to an increase in shear strength and stiffness of hydrate-free sediments.
In this study, a direct shear test model of HBS is built using the discrete element method (DEM). A series of numerical simulations with different PSD of HBS at different hydrate saturations and vertical stresses are conducted. The shear stress and vertical strain responses of HBS were analyzed and discussed based on the simulation results.

2. DEM model of HBS

2.1. Basic parameters of DEM specimens

A commercial software named PFC\textsuperscript{2D} is used in this study. Given the high computational cost of the DEM, the size of the DEM model of HBS is set to 20 mm × 20 mm. A direct shear box consisting of 8 rigid walls is created (Figure 1). Each wall of the shear box is independent. The vertical stress is applied to the top wall (Wall 5) and bottom wall (Wall 1). The shear force is applied to the side walls (e.g., Walls 2, 4, 6, and 8). Wall 3 and Wall 7 are created to prevent particles from escaping from the shear box during the movement of walls.

![Figure 1. Schematic of a shear box.](image)

The particle size distribution (PSD) of sediments is comprehensively studied in this paper. Previous studies indicate that the hosting sediments with spherical or circular shapes can behave similarly to those with irregular shapes [9]. This paper mainly focuses on the influence of the particle size distribution on the shear behavior of the HBS; therefore, only 2D circular disks are used to represent the sediment particles to simplify the DEM models. A series of PSDs of sediments are used, as shown in Figure 2. The PSDs are divided into two groups: Group 1 and Group 2. In Group 1, the median sizes of the PSDs are constant, while the uniformity coefficients (Cu) of the PSDs are different. In Group 2, the uniformity coefficients of the PSDs are set to 1 while the median sizes are different. The uniformity coefficient is defined as the following equation:

\[ Cu = \frac{D_{60}}{D_{10}} \]  

where \( D_{60} \) is the particle size which cumulative mass accounts for 60%, and \( D_{10} \) is the particle size which cumulative mass accounts for 10%.

Two-dimensional DEM simulations of direct shear box tests are used. Note that the porosity of the specimen in two-dimensional simulations differs from that in three-dimensional lab tests. The 2D porosity is much smaller than the 3D porosity. It is difficult for the conversion from two-dimensional to three-dimensional porosity. Following previous research of Ouyang and Li [10], this study uses the equations of three-dimensional-two-dimensional transformation equations for equal-sized particles. The 2D porosity corresponding to the original hosting sediments in the laboratory is 0.14 using equation 2.
where \( n_{2D} \) is two-dimensional porosity, \( n_{3D} \) is three-dimensional porosity, \( \varepsilon \) is conversion factor, and \( D_r \) is relative density.

\[
\begin{align*}
\frac{n_{2D}}{n_{3D}} &= 1 - \left(\frac{1 - n_{3D}}{\varepsilon}\right)^\frac{1}{2} \quad (n_{3D} \in [0,1], \quad n_{2D} \in [0.143,1]) \\
\varepsilon &= \frac{\sqrt{2}}{\sqrt{\pi \sqrt{3}}} + \frac{D_r}{\sqrt{2}} \left(\frac{0.606}{\sqrt{\pi \sqrt{3}}} - \frac{0.857}{\sqrt{\pi \sqrt{3}}}\right) \quad (\varepsilon \in [0.606,0.857])
\end{align*}
\]  

Figure 2. The particle size distribution in laboratory tests and numerical simulations.

The preparation of the DEM model is introduced as follows (Figure 3). First, the sediment particles following the given PSD are randomly generated in the shear box. The sediment particles do not overlap each other. Second, the generation of sediment particles is stopped when the initial porosity of the sediment reaches the target porosity. Third, the hydrate particles with a diameter of 0.05 mm are randomly generated in the remaining pores until the hydrate saturation reaches the target saturation. Finally, the pre-compaction and consolidation of the DEM specimen are performed at a given vertical stress. The vertical stresses are 0.3 MPa, 0.6 MPa, and 0.95 MPa. The hydrate saturation is defined as the ratio of the volume of hydrates to the pore volume of sediments. The DEM model of HBS has been calibrated by the authors previously. The basic parameters for the calibrated DEM model are listed in Table 1.

The relationship between the number of contact and the angle with respect to the axis is demonstrated by rose diagram in Figure 4. Figure 4 (a)-(c) indicate that the initial hosting sediments with different particle size distributions under the constant median particle size are roughly isotropic. Figure 4 (d)-(f) show that the packing of the monosized hosting sediments is anisotropic. The reason is that sediment particles turn to be dense under a given confining pressure. The monosized circular particles are rearranged to form a stable equilateral triangle structure with the adjacent particles. Therefore, the contact orientation is limited at 60-degree intervals. With the increase in particle size, the packing of the hosting sediments is more anisotropic. One of the limitations is that the particle number is not large enough since a larger number of particles requires a higher computational cost.
2.2. The contact model and mechanical parameters of DEM specimens

Since natural gas hydrate occurs in unconsolidated or low-consolidation submarine sediments, there is no cohesion between sediments. Hence, the linear contact model is used for the sediment-sediment, sediment-wall contacts.

In the linear contact model, the normal and tangential stiffnesses at the contact point are the harmonic averages of the stiffness in the two directions of the two particles. The equations are shown as follows.

\[
\begin{align*}
    k_n &= \frac{1}{\frac{1}{k_{n1}} + \frac{1}{k_{n2}}} = \frac{k_{n1}k_{n2}}{k_{n1} + k_{n2}} \\
    k_s &= \frac{1}{\frac{1}{k_{s1}} + \frac{1}{k_{s2}}} = \frac{k_{s1}k_{s2}}{k_{s1} + k_{s2}}
\end{align*}
\]  

(3)
where \( k_{n1}, \ k_{n2} \) are the normal stiffness of Particle 1 and Particle 2 respectively, \( k_{s1}, \ k_{s2} \) are the tangential stiffness of Particle 1 and Particle 2 respectively.

Although the parameters of the contact model are difficult to directly measure in the laboratory, the parameters can be calibrated by parametric analysis. After calibrating the DEM model, the mechanical parameters of the sediment particles, hydrate particles, and walls are given in Table 1. It is assumed that there is no friction between the walls and particles.

Due to the cohesive nature of hydrates, the parallel bond contact model is applied to the contacts between hydrate-hydrate and hydrate-sediment contacts. When the parallel bond contact breaks during the shearing process, a linear contact takes place of the bonded contact. After the calibration with the laboratory tests, the basic parameters of the parallel bond contact model are given in Table 2.

**Table 1.** The physical parameters of sediment particles, hydrate particles, and wall in the numerical simulation.

| Parameter                  | Notation | Soil | Hydrate | Wall | Unit       |
|----------------------------|----------|------|---------|------|------------|
| Density                    | \( \rho_h \) | 2650 | 900     | 2650 | kg/m\(^3\) |
| Normal stiffness           | \( k_n \) | \( 1.0 \times 10^8 \) | \( 1.0 \times 10^7 \) | \( 1.0 \times 10^8 \) | Pa          |
| Tangential stiffness       | \( k_s \) | \( 1.0 \times 10^8 \) | \( 1.0 \times 10^7 \) | 0.0 | Pa          |
| Effective modulus          | \( E^* \) | \( 3.0 \times 10^8 \) | \( 3.0 \times 10^8 \) | -  | Pa          |
| Coefficient of friction    | \( \mu \) | 0.5  | 0.1     | 0.5  | -          |

**Table 2.** Parameters of parallel bonds used in the DEM simulations.

| Parameters                     | Notation | Hydrate-Hydrate | Hydrate-Soil | Unit |
|--------------------------------|----------|-----------------|--------------|------|
| Tensile strength \( \sigma_{h-h} \) | \( 1.5 \times 10^7 \) | \( 1.4 \times 10^7 \) | Pa    |
| Cohesion \( c_{h-h} \)          | \( 1.5 \times 10^7 \) | \( 1.4 \times 10^7 \) | Pa    |
| Internal friction angle \( \phi_{h-h} \) | 0.0      | 0.0            | °      |

3. Results and discussion

3.1. Effect of PSD on the shear behavior of HBS

Figure 5 shows the stress-strain and the vertical strain-shear strain curves of the HBS with the hosting sediments of different uniformity coefficients (e.g., 1.177, 1.413, 1.742) at different hydrate saturations and different vertical stresses. Each test is labeled according to the uniformity coefficient and hydrate saturation. For example, PSD_S_10 means that the uniformity coefficient is relatively small (\( Cu=1.177 \)), and the hydrate saturation of the HBS model is 10%.

According to Figure 5 (a)-(c), the shear strength and dilation of HBS increase with increasing hydrate saturation and vertical stress regardless of the uniformity coefficient of the hosting sediments. This increasing trend is also consistent with the results of laboratory tests. For clean sand sediments (hydrate saturation is 0), when the median particle size and porosity are the same, the stress-strain curves of HBS are almost coincident. In this case, the particle size distribution has no significant influence on the mechanical properties of clean sand sediments. In addition, at the lower vertical stress and the same hydrate saturation, there is not much difference between the shear strength of the HBS with the hosting sediments of different particle size distribution ranges.

With the increase in vertical stress, the shear strength of the HBS with the hosting sediments of different particle size distribution ranges varied significantly when the hydrate saturation is high. The larger the uniformity coefficient of hosting sediments, the higher the shear strength of HBS. However, the dilation of HBS shows an opposite trend. According to Figure 5 (d)-(f), when the vertical stress is high, the dilation of HBS with the hosting sediments of different particle size distributions is similar at the same saturation. However, the dilation of HBS at high hydrate saturations is different when the
vertical stress is low. Overall, a more uniform PSD results in a greater dilation of HBS.

The internal friction angle and cohesion of HBS can be calculated according to the Mohr-Coulomb criterion, as shown in Figure 6. With the increase in hydrate saturation, the internal friction angle of HBS varied for different PSDs. The internal friction angle of HBS with the hosting sediments of a small uniformity coefficient increases with increasing the hydrate saturation. The degree of increase is greater for a higher hydrate saturation. When the uniformity coefficient of hosting sediments increases, the internal friction angle decreases with the increase in hydrate saturation. However, for the HBS with the hosting sediments of different PSDs, the cohesion increases with increasing hydrate saturation. The cohesions of the HBS with the hosting sediments of different PSDs are close at the same hydrate saturation. The result is different when the hydrate saturation reaches 40%. It can be concluded that a greater uniformity coefficient of the hosting sediments leads to a greater cohesion of HBS.

Figure 5. The shear stress-shear strain and vertical strain-shear strain curves of the HBS with the hosting sediments of different PSDs at different hydrate saturations and vertical stresses.

Figure 6. Cohesion and internal friction angle of the HBS with the hosting sediments of different PSDs at different hydrate saturations.
3.2. Effect of the median particle size of hosting sediments on the shear behavior of HBS

Figure 7 presents the stress-strain curves of the HBS with the hosting sediments of different grain sizes at vertical stress of 0.30MPa for varying hydrate saturations. According to Figure 7, when the original porosity of the hosting sediments and the hydrate saturation are the same, the shear strength of HBS increases significantly with the increase in the particle size of hosting sediments. In the case of lower hydrate saturation, the shear strength of the HBS with the hosting sediments of particle size of 0.644 mm is approximately the same as that of 0.344 mm. However, even in clean sand sediments, the HBS with the hosting sediments of particle size of 0.944 mm also exhibits a significantly stronger shear strength than the former cases. In addition, the shear strain of the HBS with the hosting sediments of large particle size corresponding to the peak stress is higher than that of medium and small particle sizes.

Figure 7. The shear stress-shear strain curves of the HBS with the hosting sediments of different PSDs at 0.3 MPa vertical stresses for different hydrate saturations.

Figure 8 shows the vertical strain-shear strain curve of the HBS with the hosting sediments of different particle sizes at the vertical stress of 0.30 MPa for varying hydrate saturations. It can be seen that the dilation of HBS increases significantly as the particle size of hosting sediments increases. When the hydrate saturation is higher, the dilation of the HBS with the hosting sediments of larger particle sizes tends to be the same. The reason is that when the particles are larger, it is more difficult for the sediment particles to move.

Figure 8. The shear stress-shear strain curves of the HBS with the hosting sediments of different particle sizes at 0.3 MPa vertical stress for different hydrate saturations.

Figure 9 illustrates the relationship between the shear strength and the hydrate saturation of HBS with the hosting sediments of different particle sizes. According to Figure 9, the shear strength of HBS increases with the increase in the particle size of hosting sediments. Moreover, the shear strength of HBS increases slowly with the increase in hydrate saturation at the beginning. When the hydrate saturation is greater than 20%, the increase rate of the shear strength increases. This might be related to the occurrence of hydrates. At low hydrate saturation, the presence of hydrates mainly increases the internal friction between sediment particles which results in increasing the shear strength. With increasing the hydrate saturation, the bonding effect of hydrates to the HBS gradually increases. The
contribution of the bonding effect to the shear strength of HBS is much greater than that of the friction between sediment particles.

Figure 9. The relationship between shear strength and hydrate saturation.

4. Conclusions
In this study, a direct shear test model of HBS is built using the DEM. A series of numerical simulations of HBS with the hosting sediments of different PSDs at different hydrate saturations and vertical stresses are conducted. The major conclusions are summarized as follows:

The shear strength and dilatation of HBS are not sensitive to the uniformity coefficient of hosting sediments with the same porosity and median particle size at low vertical stress. With the increase in vertical stress, the shear strength of the HBS with the hosting sediments of different PSD ranges significantly varied when the hydrate saturation is high. The internal friction angle of HBS increases for the hosting sediments of a small uniformity coefficient while decreases for a large uniformity coefficient with increasing the hydrate saturation.

The shear strength and dilatation of HBS with the hosting sediments of the same porosity can be enhanced with the increase in median particle size prominently. When the hydrate saturation is high, the dilation of the HBS with the hosting sediments of large particle sizes tends to be the same.

5. References
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