Evolution of Coordination Number of Methane Hydrate Bearing Sediments during Quasi-static Shearing

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Abstract. Quasi-static shearing of methane hydrate bearing sediments (MHBS) was investigated by performing numerical tests using distinct element method (DEM) so as to comprehensively understand mechanical properties of MHBS. Stress-strain response and dilation behaviour of numerical tests were presented and compared with that of physical experiments. And then an examination of the evolution of coordination number (CN) during shearing was also presented, as well as its relation to anisotropy of contact orientations. The research results led us to conclude that (i) DEM can effectively capture the main characteristics of strength and deformation of MHBS; (ii) Distribution of CN shows obvious heterogeneity which is closely associated with shear bands; (iii) The average CN has a strong correlation with total number of contacts, and could be further interpreted from the point of view of anisotropy of contact orientations;

1. Introduction
Methane hydrate (MH) has a carbon quantity twice more than all fossil fuels combined[1] and a wide distribution in oceanic sediments and permafrost regions, and it has been spotlighted as a potential non-conventional energy resource[2]. It is essential to comprehensively understand the mechanical characteristics of methane hydrate bearing sediments (MHBS) for hydrate recovery.

As a new type of granular material, the macroscopic responses of MHBS are closely associated with particle-scale information which experimental studies and continuum theory seldom offered. However, the particle-scale information could be examined in detail by discrete element method (DEM)[3], a numerical technique commonly used in geotechnical engineering.

In this manuscript, macromechanical characteristics of MHBS were investigated and validated using DEM and then the evolution of coordination number (CN) during shearing and its relation to anisotropy of contact orientations was examined in detail to gain some insights into the micromechanical processes occurring at the particle scale.

2. Numerical test

2.1. Preparation for numerical sample
Figure 1 shows the DEM sample with hydrate saturation of 40%. The numerical sample was generated at random in a wall frame of 12mm × 24mm, and consisted of 21109 particles, a number which was sufficient to avoid finite size effects[4]. The hydrate particles were modelled by disks with diameters of 0.06 mm, while the soil particles were in 0.1mm to 0.4mm diameter range. The linear elastic
relationship at soil-soil contacts was introduced, and the linear parallel bond model was employed for soil-hydrate contacts and hydrate-hydrate contacts considering the hydrate acting as bonding agents. An isotropic consolidation was then conducted to bring samples to equilibrium under a prescribed confining stress of 1.0MPa. Since gravity was negligible, the particle arrangement after consolidation was uniformly distributed and could be considered almost isotropic.

![Figure 1 Numerical sample of MHBS sample and its detail at pore scale.](image)

### 2.2. Contact parameters
Contact parameters chosen in numerical experiments were tentatively calibrated in order to match the macroscopic responses of physical experiments, which are given in table 1.

| Contact types               | Contact parameters           | Values     |
|-----------------------------|------------------------------|------------|
| Soil-soil contacts          | Effective modulus (N/m²)     | $2.0 \times 10^9$ |
|                             | Normal-to-shear stiffness ratio | 1.3       |
|                             | Friction coefficient         | 0.5       |
| Hydrate-soil contacts       | Effective modulus (N/m²)     | $1.0 \times 10^6$ |
|                             | Normal-to-shear stiffness ratio | 1.3       |
|                             | Friction coefficient         | 0.3       |
|                             | Bond effective modulus (N/m²) | $1.0 \times 10^6$ |
|                             | Bond normal-to-shear stiffness ratio | 1.3       |
|                             | Tensile strength (Pa)        | $5.0 \times 10^7$ |
|                             | Cohesion (Pa)                | $4.0 \times 10^6$ |
| Hydrate-hydrate contacts    | Effective modulus (N/m²)     | $1.0 \times 10^9$ |
|                             | Normal-to-shear stiffness ratio | 1.3       |
|                             | Friction coefficient         | 0.3       |
|                             | Bond effective modulus (N/m²) | $1.0 \times 10^9$ |
|                             | Bond normal-to-shear stiffness ratio | 1.3       |
|                             | Tensile strength (Pa)        | $3.0 \times 10^6$ |
|                             | Cohesion (Pa)                | $1.2 \times 10^6$ |
2.3. Boundary conditions
Deformation of the samples was controlled through four rigid walls. During the consolidation phase, the sample was loaded in a strain-controlled fashion, but the velocities of the walls were adjusted using a servo-control mechanism so that the prescribed confining stress was achieved. At the loading phase, the top and bottom walls as loading platens move vertically under a strain-controlled condition, while the lateral walls were kept in control through the servo-mechanism in order to keep the confining pressure constant. The strain rate was fixed at 0.1%/s, small enough to meet the criteria of quasi-static loading proposed by Radjai[5].

2.4. Macroscopic responses
Figure 2(a) shows the relationships between deviatoric stress and axial strain for MHBS samples with different hydrate saturations. The corresponding evolution of volumetric strain is shown in Figure 2(b). As can be seen from the figures, at least in a qualitative sense, the macro-mechanical responses of numerical experiments are typical of that obtained in laboratory experiments[6]. The shear process undergoes two characteristic phases with different mechanical behaviours, i.e. strain hardening phase, and strain softening phase. The deviatoric stress increases up to a peak strength during strain hardening phase and drops clearly in strain softening phase. The sample with higher hydrate saturation exhibits an increase in initial tangential modulus. The volumetric strain responses indicate that MHBS samples expand.

3. Coordination number
Numerical tests using DEM enable a detailed examination of the evolution of micromechanical variables at the particle scale. Coordination number is a fundamental quantity, which is used to characterize the microstructure properties in granular material. In this subsection, we present and discuss the evolution of CN during shearing and its relation to anisotropy of contact orientations to reveal some particle-scale information.

3.1. Distribution of coordination number
Figure 3 represents distribution of CN throughout the sample with hydrate saturation of 40%. As can be seen from Figure 3, the CN shows obvious heterogeneity which has a strong correlation with strain localization (or shear band). This heterogeneity starts from strain hardening phase, and fully developed in softening phase. Therefore, the heterogeneity of CN indicates a progressive failure mechanism of sample during shearing.
3.2. Evolution of coordination number

Figure 4 shows the evolution of average CN and CN inside and outside shear band during shearing. As can be seen from Figure 4(a), a sharp decrease in the average CN arises during initial phase and then a gentle decrease follows. It can be observed from Figure 4(b) that (1) the CN outside shear band is bigger than that inside shear band; (2) the CN inside shear band changes more considerably than that outside shear bands, especially in strain softening phase. Therefore, the decrease in the average CN during strain softening phase is largely attributed to the decrease of CN inside shear band.

Figure 4 Evolution of (a) average CN and (b) CN inside and outside shear bands during shearing.
3.3. Anisotropy of contact orientations

Figure 5 shows the evolution of contact numbers in samples with different hydrate saturations. It is observed that the evolution of contact numbers exhibits a similar trend of CN, indicating a close correlation of these two variables. In order to elaborate this correlation in detail, anisotropy of contact orientations during shearing is presented in Figure 6. A considerable decline in contacts parallel to the direction of minimum principal stress and a slight increase in contacts parallel to the direction of maximum principal stress is observed in strain hardening stage, which produces a concentration in the distribution of contact numbers parallel to the direction of maximum principal stress. This concentration leads to the decrease in CN in strain hardening phase. Besides that, the decrease in contacts parallel to the direction of maximum principal stress is observed during strain softening phase, which is consistent with previous founding of Rothenburg[7] that strain softening creates contacts disintegration which is a consequence of the fact that contacts parallel to the direction of maximum principal stress tend to disintegrate. This could be primarily attributed to the fully developed shear bands in samples since the CN in shear bands is encountered with a considerable decrease.

![Figure 5](image-url)

**Figure 5** Evolution of contact numbers in samples with different hydrate saturations.
Figure 6 Anisotropy of contact orientations at (a) initial state, (b) strain hardening phase (strain: 2%), (c) strain hardening phase (strain: 3%), (d) peak stress (strain: 4%), (e) strain softening phase (strain: 10%), (f) residual state (strain: 15%), where the results of samples with hydrate saturation of 25%, 40%, 55% are presented in green, yellow, and orange respectively.

4. Conclusions
Numerical tests were carried out to simulate the overall stress-strain-dilation behaviours of MHBS with different hydrate saturations, and the evolution of coordination number and its relation to anisotropy of contact orientations were examined. The conclusions can be summarized as following: at the macroscopic scale, the simulated stress-strain-dilation responses are in satisfactory agreement with that of observed in physical experiments; the heterogeneity of coordination number indicates a progressive failure mechanism of samples during shearing; the average coordination number has a close correlation with contact numbers, which can be further interpreted from the point of view of anisotropy of contact orientations.

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