DEM analysis on the triaxial behaviour of mudstone considering water disintegration

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Abstract. Mudstone is a typical type of soft rocks. It is stable and has high strength in its natural state. However, in presence of water the constituent minerals dissolve and the inter-grain bonds are weakened, which thereby greatly reduces the strength of mudstone. As one of the most prevailing geological formations in the southwestern China, understanding the mechanical behaviour of mudstone at different degrees of disintegration is of great importance to practical engineering. This paper presents a micro-mechanical analysis on the mechanical behaviour of mudstone at different degrees of disintegration using the discrete element method (DEM). The laboratory triaxial tests carried out on mudstone samples that have been merged in water for different time periods are simulated. The dissolution of minerals and weakening of bonds between grains are considered by reducing the selected input parameters of parallel bonds at random locations. Different degrees of disintegration are obtained by multiplying the selected input parameters of parallel bonds with different reducing factors. The stress-strain curves obtained using the proposed approach are in good agreements with the experimental data. The progressive failure mechanism of mudstone at different degrees of disintegration is investigated considering the characteristics of particle motion, contact variation and bond breakage. Micro-scale analysis shows that with the increasing of confining pressure, the fraction of shear breakage of parallel bonds increases but the declining rate of coordination number post peak decreases. These underlie the fundamental mechanism of the change of failure mode of mudstone from brittleness to ductileness. Regardless of its spatial locations, the majority of broken bonds for the disintegrated specimens are those bonds with reduced input parameters. And the fraction of altered bonds within the broken bonds increases with the increasing degree of disintegration. The current research provides insightful understanding of the fundamental behaviour of mudstone in the presence of water.

1. Introduction
In accordance with the fast economy development, construction of urban underground infrastructures as well as transportation systems in rural areas in the southwestern part of China is booming in recent years. There is a special type of soft rock prevailing in these regions, i.e., mudstone. It has high strength and stiffness in its dry or nature state but is prone to disintegration in the presence of water and high temperature [1-2]. Understanding the mechanical behaviour of mudstone at different degrees of integration is of great importance for the design and construction of infrastructures.
Great efforts have been devoted to investigating the influence of water on the mechanical behavior of mudstone. Zhou et al. (2005) showed that the peak strength and strength parameters of mudstone degraded in a power-law manner with increasing merging-in-water time [2]. Erguler et al. (2008) reported that the uniaxial compression strength (UCS), elastic modulus and strength parameters of rock decreased with increasing water contents [3]. Meng et al. (2009) further showed that the failure mode of mudstone changed from brittle-type to ductile-type as merging-in-water time increases [4]. Nahazanan et al. (2013) conducted triaxial compression tests on mudstone samples under dry, short-term moisture and long-term moisture conditions and concluded that the deviatoric stress of the mudstone decreased as merging-in-water time increased [5]. Different mechanisms have been proposed to explain for the disintegration phenomena of mudstone. Heggheim et al. (2004) proposed that chemical reaction between the minerals and water may be the main reason for the change of micro-structure of rocks [6]. Duan et al. (2014) proposed that the disintegration process can be linked to increasing absorption of water which leads to the propagation and percolation of interior cracks [7]. Based on CT-scanning technique on mudstone samples subjected to different dry-and-watering cycles, Yao (2014) suggested that the damage of microstructure characterized by generation of a large number of cracks should explain for the degradation of mudstone [8]. Despite these efforts, the micro-scale mechanism underlying the progressive failure mechanism of mudstone under different disintegration conditions has not yet been well understood. A possible way to tackle this issue is to conduct the discrete element method (DEM) [9] simulations. DEM has been widely adopted to simulate the mechanical behaviours of different types of rocks [10-13]. However, so far there is no practice of applying DEM to simulate the progressive failure behaviours of mudstone with different degrees of disintegration. This study firstly explored the disintegration mechanism by identifying the micro-structure of mudstone samples merged in water for different time periods using SEM, based on which a simple approach for simulating the disintegration effects using DEM was proposed. Then a series of DEM simulations were conducted to explore the progressive failure of mudstone with different degrees of disintegration.

2. Disintegration mechanism of mudstone under different moisture conditions

In order to determine the disintegration mechanism of mudstone. The mudstone samples collected from the construction site of Metro Line 2 of Nanning City, China, were merged in distilled water for different time periods. Then, a small platy piece was cut from each sample which was then dehydrated and mounted onto the storage tube of the tungsten filament scanning electron microscope from the Department of Geotechnical Engineering, Tongji University, for scanning. Scanning was performed at three different regions for each sample. Figure 1 shows the SEM images at one selected region of the mudstone after merging in water for different time periods. Note that the SEM images were magnified for 1000 times to better illustrate the micro structure. It can be seen that the surface texture as well as the micro structure changed severely due to the presence of water. The dry specimen has a quite smooth surface texture, while the minerals dissolved in water which thereby led to the appearance of cracks and isolated micro blocks. The cracks percolate with increasing opening width as dissolution continued with increasing merging time until the entire sample became disintegrated. Big gaps were observed in the sample merged in water for 1 d, indicating that the sample tended to be disintegrated with increasing merging time. The roughness of sample surface did not increase consistently with increasing merging time, which may be attributed to the random selection of sampling areas. Figure 1 also shows that the bonds between solid grains were broken and the packing was loosened, which may be due to the reduction of cohesion between solid grains. This may be because as the merging time increases, more and more water infiltrates into the interior voids of mudstone which expels the air from the voids. With increasing water content, the cohesion between solid grains reduces due to dissolution of bonding minerals and thus the solid grains detach from each other. The entire structure becomes increasingly looser, which eventually leads to the complete disintegration.
3. Triaxial tests on mudstone samples merged in water for different time periods

Triaxial compression tests were conducted on mudstone samples merged in water for three time periods, i.e., 0 h, 10 h and 30 h considering three confining stress levels ($\sigma_c = 1.0$, 2.0 and 3.0 MPa). The stress strain curves obtained in the triaxial tests are presented in Figure 2. For all the testing samples, both the stiffness and peak strength increase with increasing confining stress. Furthermore, there is a delay in appearance of failure and the stress-strain behaviour becomes more ductile as confining stress increases. The testing results are summarized in Table 2. Overall, at each confining stress level, both the strength and stiffness decrease with increasing merging-in-water time ($t$). The cohesion ($c$) and friction angle ($\phi$) can be obtained based on Mohr-Coulomb failure criterion. As Figure 3 shows, both of these two strength parameters can be correlated with the merging-in-water time in a power-law manner, indicating that mudstone is integrated more rapidly at the early stage of merging in water.

$$c = 0.74e^{-12.35t}, \quad R^2 = 0.9993 \quad (\text{Eq. 1})$$

$$\phi = 17.47e^{-9.15t} + 6.29, \quad R^2 = 0.9984 \quad (\text{Eq. 2})$$
Figure 2. Stress-strain behaviours of mudstone samples merged in water with different time periods

Table 1. Mechanical properties of mudstone samples merged in water for different time periods

| State | $\sigma_3$/MPa | $\sigma_p$/MPa | $E_r$/MPa | $c$/MPa | $\phi^o$ |
|-------|----------------|----------------|-----------|---------|---------|
| $t = 0$ h | 1.0 | 3.79 | 58.57 | 0.74 | 23.76 |
|        | 2.0 | 4.62 | 65.19 | 0.74 | 23.76 |
|        | 3.0 | 6.48 | 78.01 | 0.74 | 23.76 |
|        | 1.0 | 1.41 | 48.37 | 0.74 | 23.76 |
| $t = 10$ h | 2.0 | 1.58 | 52.87 | 0.32 | 11.63 |
|        | 3.0 | 2.42 | 60.61 | 0.32 | 11.63 |
|        | 1.0 | 0.50 | 35.66 | 0.32 | 11.63 |
| $t = 30$ h | 2.0 | 0.60 | 38.98 | 0.07 | 6.94 |
|        | 3.0 | 1.05 | 42.34 | 0.07 | 6.94 |

Figure 3. Variation of strength parameters with water merging time

4. DEM Simulation

In order to investigate the micro-mechanics underlying the stress-strain behaviour of mudstone with different degrees of disintegration, a series of DEM simulations were conducted. Simulation setup

Figure 4 shows the configuration of DEM samples during the simulation. We adopted the radius expansion method to generate the sample as it has been reported that the DEM samples generated by this method are homogeneous and isotropic [14]. The particles whose diameter were reduced by $m$ times were initially within a cylindrical domain of $\Phi 50 \times 100$mm. The particles were then gradually expanded until the target sizes were reached. The radius reduction factor $m$ can be calculated using the formula below:
where \( n_0 \) is the initial sample porosity and \( n \) is the target porosity of 0.35. The final particle radiuses lay between 1.0 mm and 1.66 mm. The generated specimen was isotropically compressed until the prescribed confining pressure has been reached. The specimen was then subjected to triaxial shearing by simultaneously moving the top and bottom loading plates at a constant velocity until failure occurred, while at the mean time the confining pressure was maintained constant by continuously adjusting the diameter of the cylindrical wall according to the difference between the average particle-wall contact stress at the boundary and the target confining pressure. At the sample generation stage, only linear contact model was activated. Once the specimen has been generated, the contact model was swapped to the parallel model.

As elucidated in Section 2, the major mechanism of mudstone disintegration is debonding and reduction of bond strength. In order to mimic this mechanism, the input parallel bond parameters were deducted at random locations following Gauss distribution. We did not reduce the bonding parameters for all contacts as the real process of minerals dissolution is progressive and may not propagate through the specimen. Figure 4 (b) and (c) compare the bonding within the middle slice of the specimen before and after bond degradation. The number within the brackets of the figure legend indicates the number of contacts within the middle slice and different colours were used to represent bonds with different magnitudes of bonding strength. The calibrated input parameters are given in Table 2. Calibration was based on the empirical multi-variable correlations between the input parameters of parallel bond and macro stress-strain behaviour established by Jia [15] taking Young’s modulus, Poisson’s ratio, peak strength and peak strain as reference variables.

![Figure 4. Setup of DEM simulations](image)

**Table 2.** Calibrated input parameters for DEM simulations

| Input parameters                              | Unit       | Benchmark Value | Reduced value  |
|-----------------------------------------------|------------|-----------------|----------------|
|                                               |            |                 | \( t=10h \)    | \( t=30h \)    |
| Effective modulus                            | MPa        | 60.70           | 25             | 15             |
| Normal-to-shear stiffness ratio               | —          | 3.49            | 10             | 10             |
| Effective modulus of parallel bond            | MPa        | 60.70           | 25             | 15             |
| Normal-to-shear stiffness ratio of parallel bond| —          | 3.49            | 3.49           | 3.49           |
| Normal strength of parallel bond              | MPa        | 0.68            | 0.02           | 0.01           |
| Cohesion of parallel bond                     | MPa        | 1.00            | 0.06           | 0.02           |
| Friction angle of parallel bond               | °          | 0               | 0              | 0              |
| Friction coefficient                          | —          | 0.5             | 0.5            | 0.5            |
4.2 Macro-scale stress-strain behavior

Figure 5 compares the DEM simulation results with experimental data for mudstone samples with different degrees of disintegration under different confining pressures. It can be seen that for all the samples considered the DEM simulation results converge with the experimental data before the peak state. The DEM simulation results are more brittle and deviate more from the experimental curves after the peak state. The reasons for the discrepancies may be two-fold: firstly, the calibration process considers only the pre-peak variables but does not involve the post-peak responses; secondly, there are no inherent fissures or cracks inside the DEM specimen, therefore, the stress-strain behaviour obtained in DEM simulation of nature sample is more rigid and brittle post peak state. In contrast, for the disintegrated samples whose parallel bond parameters have been deducted, the stress-strain behaviours obtained in DEM simulations become more ductile than the experimental data. Despite these discrepancies, the closeness between the DEM simulation results and experimental data are remarkable, which indicates that our proposed method of simulating the disintegration of mudstone when merging in water is effective.

![Figure 5. Comparing the DEM simulation results with experimental data under different degrees of disintegration](image)

4.3 Microscopic analysis of the progressive failure mechanism

The failure process of rock materials is characterized by generation and coalescence of cracks, which can be reflected from the bond breakage events in DEM simulations. For natural sample under confining pressure of 1.0 MPa, as Figure 6 shows, bond breakage events are rare and concentrated at the two ends of the sample at the initial stages of loading as loading velocity was applied at the top and bottom rigid walls. With the further increase of axial load, the mudstone specimen starts to expand laterally, therefore, cracks are formed in the middle part of the sample. As loading proceeds, the cracking events accelerate
and apparent shear bands are formed at the peak state due to the coalescence of micro cracks. Bonds continue to break and propagate throughout the entire sample post peak, which thereby cause the final failure. In contrast, at a higher confining pressure, no apparent shear bands are observed. The broken bonds percolate in the middle central part of the sample, in accordance with the lateral plastic expansion deformation pattern observed experimentally [14]. The failure process for other samples is similar to Figure 6 and thus is not presented for conciseness. The bond could fail either in tension or by shear. As shown by Jia [15], bond breakage is dominated by tension when the confining pressure is low. In contrast, Figure 7 shows that when the confining pressure exceeds 1.0 MPa, shear failure will be the dominating failure mechanism. As Figure 7 shows, for all the three mudstone samples, the cracking process can be divided into three stages: a stable stage at which a small number of bonds break; an accelerating stage at which the bond breakage rate increases rapidly when approaching the peak state; and a decelerating stage when the bond breakage rate decreases post peak. The total number of failed bonds increases with increasing merging-in-water time and there are fewer bonds failed in tension as the merging-in-water time increases, but the increasing rate of failed bond decreases with increasing merging-in-water time. 70% of the failed bonds belong to the degraded bonds for the sample merged in water for 10 h, while 73% of the failure bonds belong to the degraded bonds for the sample merged in water for 30 h, indicating that the degraded bonds will become more dominating as the degree of disintegration increases.
Figure 6. Distribution of failed bonds at different stages of natural mudstone sample under a confining pressure of (a) 1.0 MPa; (b) 3.0 MPa.
Figure 7. Evolution of the number of broken bonds for mudstone samples with different merging-in-water time under a confining pressure of 1.0 MPa

The broken event as well as the progressive failure process can also be inferred from the evolution of coordination number (CN), which is defined as:

\[ CN = \frac{1}{N_p} \sum_{i=1}^{N_p} N^c_i \]  

(Eq. 4)

where \( N_p \) and \( N^c_i \) are the total number of particles and the number of contacts owned by particle \( i \), respectively. As shown in Figure 8, for the natural sample, at all confining stress levels CN remains approximately constant at initial stages of loading but it drops abruptly at the peak state. With increasing confining pressure, the drop of CN post peak becomes gentler. For the merged-in-water samples, CN drops at instants earlier than the peak and the declining trend is less steep than the natural sample, in accordance with Figure 7 which shows that the bond breakage rate is higher for sample at the natural state than that for the merged-in-water samples. Note that the overall trend for \( \sigma_c=2.0 \) MPa case is similar to \( \sigma_c=1.0 \) MPa case, therefore, they are not presented but are substituted by the data with a smaller \( \sigma_c=0.1 \) MPa.

Figure 8. Evolution of coordination number during triaxial simulations on mudstone samples with different merging-in-water time periods

Conclusion

In this paper, the micro-scale mechanism underlying the disintegration of mudstone in presence of water was firstly explored using SEM technique. It was found that disintegration of mudstone could be mainly attributed to debonding and reduction of cohesion due to the dissolution of minerals. Based on this mechanism, an approach of simulating the mechanical behaviour of mudstone with different merging-
in-water time was proposed by deducting the parallel bond parameters at random locations. It was shown that the proposed approach could effectively capture the mechanical responses of mudstone samples with different degrees of disintegration. Micro-scale analyses further showed that the progressive failure of mudstone could be closely linked to the bond breakage events and evolution of coordination number. Since in real situation dissolution of minerals and debonding may propagate from exterior area to inner area of rock specimens, the current approach needs to be improved by considering the spatial disparity of distributions of both broken bonds and bonding parameters.

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Acknowledgments
The work was supported by the National Natural Science Foundation of China (Grant No. 41672262).