DEM simulation of the complete triaxial test of sandstone

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Abstract. Complete triaxial tests considering residual strength are of great significance in analyses of the mechanical properties of rock in deep-rock engineering. In this paper, the complete triaxial test of Berea sandstone was quantitatively simulated using the discrete element method. The macro- and micromechanical properties of Berea sandstone were analyzed, and the following conclusions were obtained: (1) As the confining pressure increases, the peak and residual strengths of the sample increases, the stress–strain curves gradually change from softening to hardening, and the volume curves gradually change from dilatancy to shrinkage. (2) When the confining pressure is low, bond failure between particles mainly occurs under the state of tensile stress. As the confining pressure increases, compressive state failure gradually exceeds tensile state failure. (3) Under different confining pressures, the energy dissipated by friction between particles is far greater than other forms of energy dissipation and the energy dissipated by rolling between particles is always greater than the energy dissipated by twisting.

1. Introduction
The discrete element method (DEM) is a numerical strategy for analyzing granular materials proposed by Cundall and Strack in 1979 [1]. The method is based on the contact model and Newton’s second law and used to solve the force and motion equations of each particle in a material. Because this method does not depend on the macroconstituents of materials, it presents significant advantages over other methods in the analysis of large deformation, discontinuity, failure, and dynamic problems. DEM is a powerful tool used to evaluate the mechanical properties of geotechnical materials. It can continuously observe and record micro information within a sample, thereby facilitating the study of the mechanical properties of granular materials from the micro to the macro scale [2,3]. In this study, DEM was combined with an improved 3D bond model incorporating rolling and twisting resistances to simulate the macro- and micromechanical properties of Berea sandstone via a complete conventional triaxial test under a wide range of confining pressures.

2. Contact model
An improved 3D bond model incorporating rolling and twisting resistances [4] was employed in this study. The contact model includes two components: the mechanical responses between particles and the bond strength criterion. When particles come into contact with each other, the corresponding
contact stress is assumed by both particles and their bond, and the relationship between the particles and the bond is in parallel. When a gap exists between particles, the contact stress is borne by the bond, and the relationship between the particles and the bond is in series. Details of the mechanical responses between particles [5] and the bond strength criterion [6,7] can be referenced in the literature.

2.1. Mechanical responses between particles

![Mechanical responses between particles](image)

Figure 1. Mechanical responses between particles\(^{[5]}\) in the (a) normal direction, (b) tangential direction, (c) rolling direction, and (d) twisting direction.

Figure 1 illustrates the mechanical responses between particles in the normal, tangential, rolling, and twisting directions. Here, the rolling and twisting resistances reflect the effects of the shape of the actual particles. \(K_1\) is the normal stiffness, \(K_r\) is the tangential stiffness, \(K_t\) is the twisting stiffness, \(r_s\) is the shape radius, \(K_{r_s}\) is the twisting stiffness, \(\mu\) is the friction coefficient of a particle, \(\mu_{n}\) is the overlap between particles, \(\mu_{s}\) is the relative tangential displacement, \(\theta_r\) is the relative rolling angle, \(\theta_t\) is the relative twisting angle, \(F_n\) is the normal force, \(F_s\) is the tangential force, \(M_r\) is the rolling moment, and \(M_t\) is the twisting moment.

2.2. Bond strength criterion

In the DEM simulations, the bond between particles is approximated as a cylinder with a height equal to the sum of the radii of the two contacting spheres. The bond is assumed to be ideal elastic brittleness. When the load exceeds the strength envelope in the shear–rolling–twisting space incorporating the normal force, the bond breaks and completely loses its strength. The formulation of the bond strength criterion is given in the literature [6,7]. Figure 2 illustrates the bond strength criterion in the DEM simulation; here, \(R_s\), \(R_r\), and \(R_t\) are the absolute values of the shear, rolling, and twisting resistances, respectively, \(F_s\) is the shear force, \(M_r\) is the rolling moment, \(M_t\) is the twisting moment, \(F_n\) is the normal force, \(A_b\) is the area of the bond, \(\sigma_t\) is the unit tensile strength of the bond, and \(\sigma_c\) is the unit compressive strength of the bond.
3. DEM simulation of the triaxial tests

3.1 Sample preparation

As shown in Figure 3, the sample is cubic in shape and has 40,206 particles. The object of the DEM simulation is Berea sandstone in a deep stratum\textsuperscript{[8,9]}. Details for parameter calibration can be referenced in the literature\textsuperscript{[4]} and are list in Table 1. The sample fist was generated by the multi-layer undercompaction method\textsuperscript{[10]} with a target void ratio of $e = 0.8$. Subsequently, a vertical pressure of 30 MPa was applied to the sample under the $K_0$ stress path to reproduce the natural deposition of particles in the deep stratum. When the stress of the sample had stabilized, bonds were generated where the gap between particles is less than the bond thickness $g_c$, and the sample was unloaded to an isotropic stress of 1.0 kPa to simulate the sampling process in situ. Finally, the sample was used in simulated triaxial
3.2 Macroscopic mechanical behavior

Figure 4 presents the results of the triaxial tests obtained from DEM simulations and laboratory experiments. The curves obtained from DEM are generally consistent with the results of the laboratory experiments, thus proving that DEM simulation could quantitatively simulate the complete process of triaxial tests of Berea sandstone.

Figure 4 shows changes in the stress and volume as a function of the axial strain during triaxial tests under high confining stresses. As the confining pressure increases, the peak and residual strengths of the sample increase and the stress–strain curve of the sample gradually changes from softening to hardening. That is to say, as the confining pressure increases, the deformation characteristics of Berea sandstone change from brittleness to ductility, and the volume change curve gradually changes from dilatancy to shrinkage. When the strain reaches 15%, the stress–strain curve is basically stable; similarly, when the strain reaches 20%, the volume change curve is basically stable. The confining pressure of brittle–ductile transition is 40–140 MPa, and the condition of brittle–ductile transition is \( \sigma_0/\sigma_3 = 3.34–5.8 \).

![Graph showing stress-strain relationship](image)

**Fig. 4** Comparison of the results of conventional triaxial tests obtained from laboratory experiments and DEM simulations in this study.

3.3. Bond failure

This paper systematically classifies the failure modes of micro bonds on the basis of the improved bond contact model. First, bond failure can be categorized according to the normal stress state of bonds into compressive state failure and tensile state failure. If the bond normal stress when bond failure occurs is of the compressive type, the bond failure type is called compressive state failure; if the bond normal stress is of the tensile type, the bond failure type is called tensile state failure. Second, the bond failure form could be categorized according to the coupling strength envelope of the bond into shear failure, rolling failure, and twisting failure. Here, the shear term with the largest proportion is called shear failure, the rolling term with the largest proportion is called rolling failure, and the twisting term with the largest proportion is called twisting failure. Combining the two classification methods described above, bond failures could be divided into shear, rolling, or twisting failure under compressive stress and shear, rolling, or twisting failure under tensile stress. The six forms of bond failure are compressive shear (CS), compressive rolling (CR), compressive twisting (CT), tensile shear (TS), tensile rolling (TR) and tensile twisting (TT), and the sum of CS, CR, and CT equals the compressive state failure. In addition, the sum of TS, TR, and TT equals the tensile state failure.

As shown in Figure 5, when the confining pressure is low (e.g., 10 and 20 MPa), the bond failure mode is mainly tensile state failure. As the confining pressure increases, compressive state failure gradually exceeds tensile state failure and the growth curve of the number of bond failures first
increases rapidly and then stabilizes. This result indicates that bond failure occurs intensively and suddenly when the confining pressure is low. Regardless if the confining pressure is high or low, during tensile state failure, the main failure mode is always TR failure, followed by TS failure, and then TT failure. When the confining pressure is 10 MPa, the main form of compressive state failure is CR failure, followed by CS failure, and then CT failure. As the confining pressure increases, the main form of failure gradually transitions to CS failure, the proportion of CS failure gradually increases, and the growth rate of the number of bond failures gradually decreases.

![Graphs showing bond failure law under different confining pressures](image)

**Figure 5** Bond failure law.

### 3.4. Energy conversion

As shown in Figures 6, 7, and 8, the particle friction dissipation energy (PFDE) is far greater than other forms of energy dissipation under different confining pressures, i.e., most of the work by the wall (WW) is ultimately converted into PFDE, and the particle rolling dissipation energy (PRDE) is always greater than the particle twisting dissipation energy (PTDE).

When the confining pressure is low, the particle elastic energy (PEE) increases rapidly to a peak value and then decreases gradually until it stabilizes. When the confining pressure is high, the PEE increases with increasing strain but the increase speed decreases gradually.

As the strain increases, the bond elastic energy (BEE) first increases and then decreases until it gradually approaches zero. According to the previous bond failure curve, bond failure is rare in the initial stages of loading. Thus, the BEE increases with increasing strain. When the strain exceeds a certain value, bond failure significantly increases and the sample enters the plastic deformation stage. Thus, the BEE begins to decrease.

When a bond breaks, the BEE transforms into bond failure energy (BFE), i.e., the BFE is the superposition of BEE in the critical failure state of the bond. The BFE develops steadily with increasing strain at the initial loading stage and then increases rapidly until it finally stabilizes.

The damping dissipation energy (DDE) is close to zero at the initial loading stage and does not increase significantly with increasing strain. Further increases in strain bring about rapid increases in the BFE and DDE.

The particle kinetic energy is close to zero in all cases, thereby indicating that the sample is loaded sufficiently slowly to meet quasi-static loading conditions.
4. Conclusions
The macro- and micromechanical properties of sandstone were analyzed over a wide range of confining pressures in a complete triaxial test. The main conclusions are as follows:

(1) As the confining pressure increases, the peak and residual strengths of the sample increase, the stress–strain curve of the sample gradually changes from softening to hardening, and the volume change curve gradually changes from dilatancy to shrinkage. The condition of brittle–ductile transition is $\sigma_1/\sigma_3 = 3.34–5.8$.

(2) When the confining pressure is low, the bond failure is mainly tensile state failure. As the confining pressure increases, compressive state failure gradually exceeds tensile state failure. The main failure mode for tensile state failure is always TR failure, followed by TS failure, and then TT failure. When the confining pressure is 10 MPa, the main form of compressive state failure is CR failure. As the confining pressure increases, the main form of failure gradually transitions to CS failure.

(3) Under different confining pressures, the PFDE is far greater than other forms of energy dissipation, and the PRDE is greater than the PTDE. In the elastic stage, WW is mainly transformed into PEE and BEE. After entering the plastic stage, all forms of energy dissipation increase synchronously and rapidly. Continuous increases in strain convert WW into the PFDE.

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References

[1] Cundall P A, Strack O D L 1979 A discrete numerical model for granular assemblies Geotechnique 29 47-65
[2] Hoek E, Martin C 2014 Fracture initiation and propagation in intact rock—a review J. Rock Mech. Geotech. Eng. 6 287-300
[3] Lisjak A, Grasselli G 2014 A review of discrete modeling techniques for fracturing processes in discontinuous rock masses J. Rock Mech. Geotech. Eng. 6 301-314
[4] Li L, Jiang M J, Liu F 2018 Calibration of a Distinct Element Model for Rock Considering the Residual Strength Pro. GeoShanghai 2018 Int. Conf.: Rock Mech. Rock Engi. 48-56
[5] Jiang M J, Shen Z F, Wang J F 2015 A novel three-dimensional contact model for granulates incorporating rolling and twisting resistances. Comput. Geotech. 65 147-163
[6] Li L, Jiang M J, Zhang F G 2018 Quantitative simulation of the triaxial test considering residual strength on the deep rock using DEM and parameters analysis. Rock Soil Mech. 39 1082-1090 (in Chinese)
[7] Shen Z F, Jiang M J, Wan R 2016 Numerical study of inter-particle bond failure by 3D discrete element method Int. J. Numer. Anal. Met. 40 523-545
[8] Rutter E H, Glover C T 2012 The deformation of porous sandstones; are Byerlee friction and the critical state line equivalent? J. Struct. Geol. 44 129-140
[9] Bera B, Mitra S K, Vick D 2011 Understanding the micro structure of Berea Sandstone by the simultaneous use of micro-computed tomography (micro-CT) and focused ion beam-scanning electron microscopy (FIB-SEM). Micron 42 412-418
[10] Jiang M J, Konrad J, Leroueil S 2003 An efficient technique for generating homogeneous specimens for DEM studies. Comput. Geotech. 2003, 30 579-597