Stochastic structural model of rock and soil aggregates by continuum-based discrete element method

WANG Yuannian[1], ZHAO Manhong[1], LI Shihai[1] & J.G. Wang[2]

1. Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China;
2. Tropical Marine Science Institute, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260

Correspondence should be addressed to Li Shihai (email: shli@imech.ac.cn)

Received April 5, 2005

Abstract This paper first presents a stochastic structural model to describe the random geometrical features of rock and soil aggregates. The stochastic structural model uses mixture ratio, rock size and rock shape to construct the microstructures of aggregates, and introduces two types of structural elements (block element and jointed element) and three types of material elements (rock element, soil element, and weaker jointed element) for this microstructure. Then, continuum-based discrete element method is used to study the deformation and failure mechanism of rock and soil aggregate through a series of loading tests. It is found that the stress-strain curve of rock and soil aggregates is nonlinear, and the failure is usually initialized from weaker jointed elements. Finally, some factors such as mixture ratio, rock size and rock shape are studied in detail. The numerical results are in good agreement with *in situ* test. Therefore, current model is effective for simulating the mechanical behaviors of rock and soil aggregates.

Keywords: CDEM, rock and soil aggregate, mixture ratio.

DOI: 10.1360/04zze13

Ancient slope[1], debris-flow deposit[2] and rock-filling dam[3] are usually made of rock and soil aggregates (RSA). The RSA is a typical inhomogeneous and discontinuous medium, and its main characteristics include: (i) loose piling up by blocks or particles, (ii) mixing of different blocks with a range of shapes and sizes, (iii) stochastic distribution of blocks in space, (4) fillings often in between blocks. The mechanical properties of these rock and soil aggregates are commonly obtained by large-scale experiments[1]. Large-scale experiments are usually expensive. Small-size laboratory tests are an alternative to measure the mechanical characteristics of rock blocks and fillings. Some homogenization theories such as homogenization method[4] are then developed to get the macro-mechanical properties of rock and soil aggregates. This paper uses a continuum-based discrete element method (CDEM) to simulate the mechanical characteristics of the aggregate of "rock and soil" through a microstructural model constructed from stochastic models.

A lot of publications have focused on the modeling of stochastic characteristics of geologic materials. Axelrad[5] systematically treated the stochastic evolvement and probability of statistic model with discrete media. He summarized molecular dynamics model, grid model, and filter model as statistic models based on strict theoretical analysis such as topological approach and stochastic processes of energy. However, these models aim only at the microstructure of materials. They are hardly applicable to the evolution of rock and soil aggregates because the microstructural evolution of RSA is more complex and uncertain. Einstein and his colleagues presented an MIT stochastic model to represent the fracture patterns of geologic materials. The MIT stochastic model was applied to describe the joints characteristic of rock mass in Boston area[6]. It can describe four stochastic processes including the orientation of joint planes, connecting and the spatial degree of fissure. However, the MIT model depends only on the presentation of geometric and geologic characteristics. The effect of the evolution of microstructures on the mechanical characteristics is not involved.

This paper proposes a stochastic model for constructing the microstructural model for CDEM with mixture ratio, rock size and rock shape as the geometrical features. It can more exactly represent the geometrical features of rock and soil aggregate distributions which are usually to be obtained through geological investigation and statistics. The microstructure evolutions, such as deformation and failure, are simulated through the CDEM developed by the authors[7,8]. The internal stress and deformation of rock and soil aggregate in uniaxial loading tests are simulated and compared for different mixture ratios with or without failure. Finally, the failure mode in a large-scale *in situ* test is reproduced using the current method.

1 Mechanical model and numerical approach to CDEM

1.1 Concept of CDEM

The mechanical model is based on the CDEM which combines finite element method (FEM) and particle-spring model[7,8] in discrete element method (DEM)[9,10]. This CDEM treats an 8-node solid isoparametric element in FEM as a fundamental system composed of 8 particles and interconnecting springs as shown in Fig. 1. The particle mass is determined by material density and its spatial distribution. The stiffness matrix of this fundamental system is the same as the element stiffness matrix of 8-node solid isoparametric element. We divide this stiffness matrix into 3×3 stiffness sub-matrix to determine the spring stiffness. That is, if three eigenvalues of the 3×3 stiffness sub-matrix are all real, two particles are connected by three springs, and the magnitude of springs is equal to the eigenvalue and the directions of springs are along the eigenvectors. If there are two conjugate eigenvalues, the elastic body between two particles is presented by five rather than three springs in three directions, among which two have

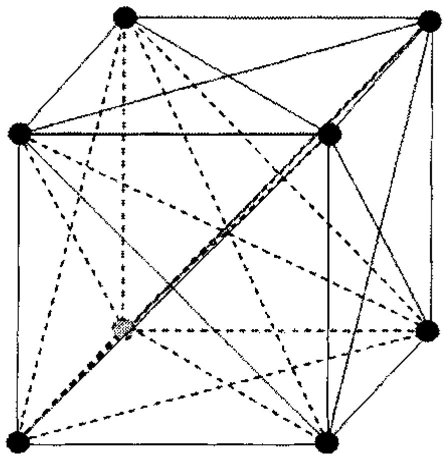

Fig. 1. Sketch of particles and springs.

Poisson effect. Whether three-springs or five-springs exist, the stiffness matrix of each fundamental system is the same as element stiffness in FEM if the material is continuous. Furthermore, the breakage of springs is used to describe the evolution from continuous to discontinuous deformations under loading or a micro-failure process. Thus, the CDEM can describe a complete process from continuous to discontinuous deformations. The criterion of spring breakage is directly associated with the strength of material. After breakage, the relevant eigenvalue is set at zero. After coordinate transformation for updated local stiffness matrix, a stiffness matrix in global coordinates is obtained.

A microstructural model of rock and soil aggregates has two types of structural elements, namely block element and jointed element, as seen in Fig. 2, and three types of material elements, namely rock element, soil element, and weaker jointed element. Combination of these elements can enable us to describe the spatial distribution of rock and soil aggregates. Jointed elements lie between block elements which are a bit thinner

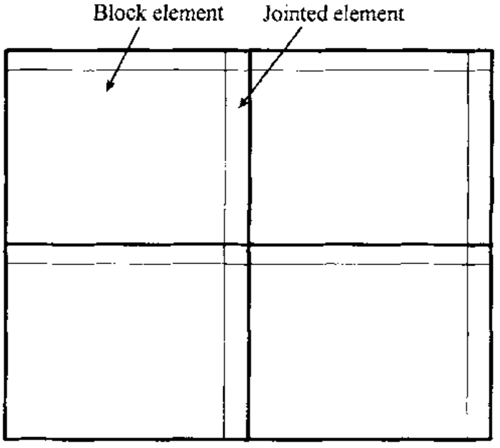

Fig. 2. Sketch of structural elements (2 dimensions).

than block elements. A jointed element between rock block element and soil block element are called a weaker jointed element which has a relatively poor strength, while those jointed elements between rock block elements as well as between soil block elements have the same material parameters as rock or soil element.

Some basic assumptions are made for this microstructural model. (i) the mechanical characteristics of block rock or filling soil are known; (ii) each rock or soil block is made up of a cluster of small block elements which have the same mechanical characteristics; (iii) the mechanical parameters of jointed element have three types: between rock block elements, between soil block elements, and between rock and soil block elements; (iv) the strength of each element is relevant to its deformation modulus; (v) the deformation of each block element is obtained according to the state of stress and constitutive relation of materials.

1.2 Failure criterion

The spring can be broken if the tensile strength or the compressive shear strength is satisfied. The tensile strength can be expressed as $\varepsilon_n > \varepsilon_0$, where $\varepsilon_n = \Delta L_n / L$. L is the distance between two nodes and ΔL_n is its increment. The compressive shear strength is described by the Mohr-Coulomb law in the spring direction. The typical strength is $\varepsilon_\tau > \varepsilon_{\tau 0} = (1+\mu)\left(\frac{C}{E} + \varepsilon_n \mathrm{tg}\varphi\right)$, where C, φ are the strength parameters, μ is the Poisson ratio and E the Young's modulus. Subscript 'r' refers to the shear direction. Therefore, the spring can be broken by either tension or compressive shear force. Because one node has at least three springs, it is expected that the current CDEM can more accurately describe the micro-failure process under any loading path.

2 Construction of CDEM microstructure by stochastic model

2.1 Mixture ratio and distribution of rock and soil blocks

CDEM uses parallel-piped block elements in computation. These block elements are obtained by intersection of three sets of joint planes. Here we will present a stochastic method to construct block elements with the above three geometrical features. For the mixture ratio of a rock, we distribute rock and soil block elements as follows: We give each block element a value between 0 and 1, and take the function $F(x) = x$ as a uniform distribution function ranging from 0 to 1. If the mixture ratio of the rock is ω, a separating value A is defined as $A = \omega/(1+\omega)$. We then mark rock and soil block elements by taking a stochastic value x between 0 and 1. If $F(x)$ is smaller than A, the block element is rock, otherwise, the block element is soil. As an example, when the mixture ratio is 1:4 in an area, the separating value A=0.25/ (1+0.25) =0.2. For one block element, if the stochastic value is x =0.3 or $F(x)$ =0.3, because it is greater than 0.2. This block element is defined as soil. After marking all block elements, the distribution of rock and soil block element is determined for the mixture ratio of 1:4.

2.2 Scale of block size

There are myriads of changes in the size and shape of rock block on a site. According to mixture ratio, the distribution of rock and soil element is determined in the last step. Element size in the last step cannot reflect the lump characteristic of rock. In order to make the rock size close to real rock, the following treatment is proposed in this paper: Divide the whole research area into numbers of sub-areas, and let the three dimensions of sub-area be consistent with maximum and minimum lengths of rock in stochastic meaning. If the numbers of layers in three dimensions of a sub-area are L_i, L_j, L_k respectively, the total block elements within each sub-area (M_T) are $L_i \times L_j \times L_k$. Assemblage of all elements in the sub-area forms a rock block. The maximum of block dimensions is the largest among L_i, L_j, L_k. The volumes or total numbers (M_R) of the rock block are the numbers of rock elements in the sub-area.

2.3 Shape of above scaled block

For the same number M_R, different assemblages form different block shapes. Denote by the parameters (N_1, N_2, and N_3) the maximum numbers in three different directions. They should be generated randomly. A specific method is as follows:

$$\begin{cases} m_1 = [M_R / (L_j * L_k)] \\ m_2 = [M_R / (N_1 * L_k)] \\ m_3 = [M_R / (N_1 * N_2)] \end{cases} \rightarrow \begin{cases} N_1 = \mathrm{getstoc}(m_1, L_i) \\ N_2 = \mathrm{getstoc}(m_2, L_j) \\ N_3 = m_3 \end{cases}$$

[ ] means taking the value itself when the number inside [ ] is an integer, otherwise taking the value as rounding the number inside [ ] plus 1; getstoc(m,n) is a function that generates an integer between m and n randomly.

2.4 Direction of above shaped blocks

In practice, the shapes of rock mass vary greatly. In order to describe the rock mass more accurately, stochastically select one corner point of parallelepiped sub-area as the starting point to arrange the elements. After arranging the whole rock block elements (M_R) corresponding to N_1, N_2, N_3, stochastically collecting rock block elements is completed in this sub-area. Beside rock block elements, other block elements in this sub-area are marked as soil block elements. When finishing the collection in all sub-areas, stochastical collecting of rock block elements is accomplished in the whole research area. Some sub-areas may not be full of real blocks. At this time, the total real blocks (M_A) in sub-area are given for judgement.

2.5 Physical parameters of block elements and jointed elements

Physical parameters for different blocks and jointed elements include: geometric parameters, density, elastic modulus, Poisson ratio and strength parameters of block and jointed elements. The computational flowchart of the above stochastic model is given in Fig. 3.

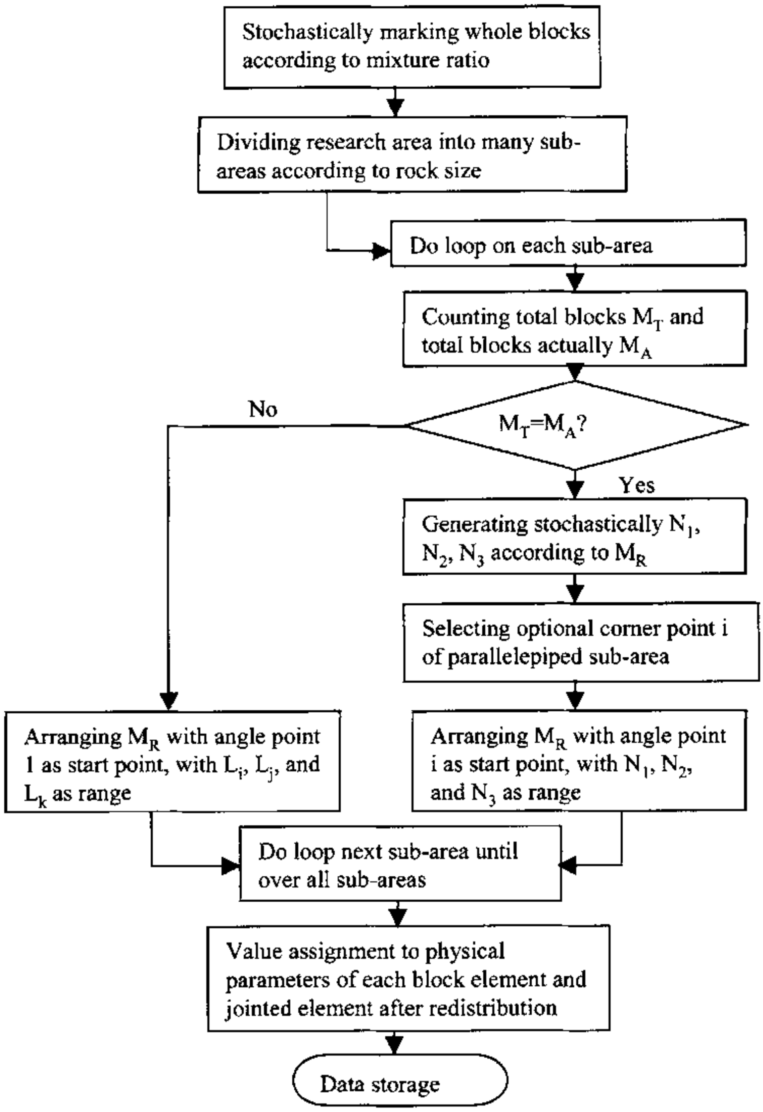

Fig. 3. Algorithm flowchart for stochastic model.

3 Simulation results on the distribution

3.1 Mixture ratio

An example is demonstrated to validate the number of rock block elements for a mixture ratio. In this example, the research volume is 20 m×20 m×20 m, the space of crosscut joint is 1 m, and the mixture ratio (rock to soil) is 1∶4. Table 1 gives the numbers of rock block elements generated in different stochastic processes. The obtained mixture ratio is approximately 20%.

3.2 Distribution of rock block element

Fig. 4 shows several typical configurations of rock elements (represented by block

Table 1 Computing results of stochastic distribution with the mixture ratio

Stochastic processes	Total block elements NT	Total rock block elements NR	NR/NT (A)
1	8000	1583	19.79%
2	8000	1596	20.00%
3	8000	1567	19.59%
4	8000	1619	20.24%
5	8000	1625	20.31%

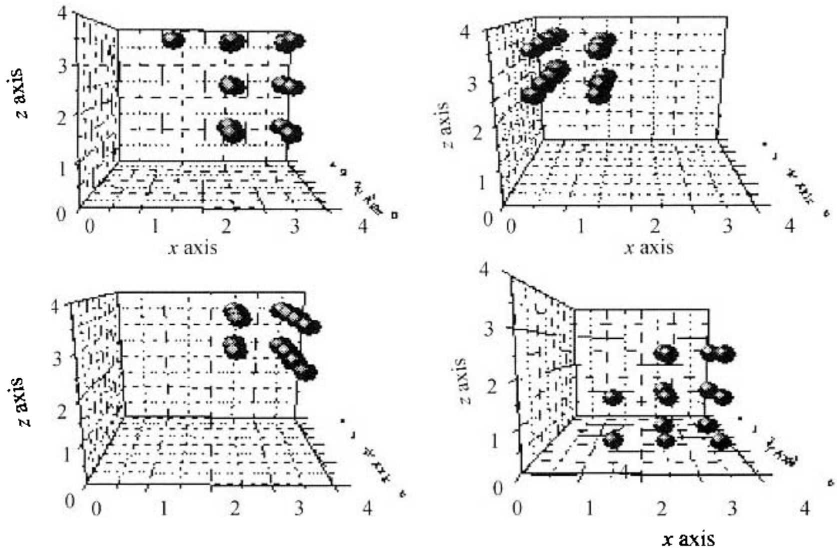

Fig. 4. Distribution of rock block elements in different stochastic processes (at the same mixture ratio).

centroids) and crosscut joints with a 4×4×4 sub-area. The mixture ratio (of rock to soil) is 1:4. Fig. 5 shows the centroid distribution of rock block elements on a cross section x=20.5 m with a 4×4×4 sub-area within a 40m×60m×80m research area. Computational results show that the model of stochastic distribution can well describe the local geologic condition for rock and soil aggregates.

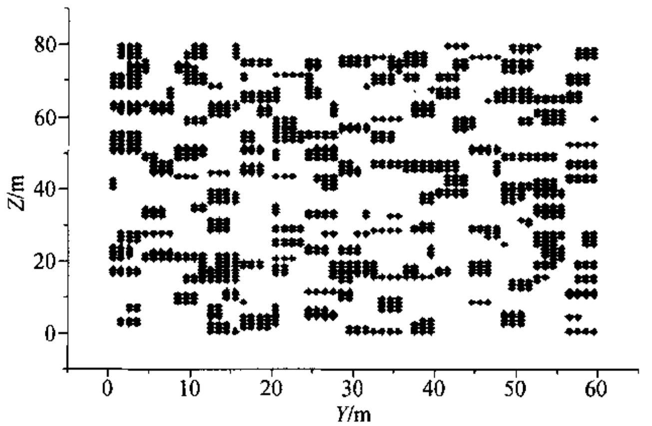

Fig. 5. Distribution of rock block elements in one cross section (40% rock).

4 Numerical simulation for uniaxial loading test

4.1 Computation parameters

The material parameters of a weaker jointed element can be obtained from the following deformation equivalence of rock element and soil element: If the elastic modulus and Poisson ratio are E_r, ν_r for rock element and E_s, ν_s for soil element, elastic modulus and Poisson ratio for a weaker jointed element is obtained as $E_w = \dfrac{2E_r \cdot E_s}{E_r + E_s}$ and $\nu_w = \dfrac{\nu_r \cdot E_s + \nu_s \cdot E_r}{E_r + E_s}$. Table 2 lists the computation parameters used.

Table 2 Physical parameters for computation

Material element	Elastic modulus/GPa	Poisson ratio
Rock element	20	0.2
Soil element	0.3	0.35
Weaker jointed element	0.6	0.347

4.2 Elastic simulation for uniaxial loading

In the following simulations, the research area is 4 m×4 m×4 m and the uniaxial load is 1 MPa. The loading is applied to the top surface and the bottom is fixed. Fig. 6 shows the contour of displacement on a y = 2.0 m section for two mixture ratios. When aggregates are all soils, or the materials are homogeneous, the contour of displacement is nearly parallel. However, the contour of displacement is anomalous if the aggregate has 20% rock. Fig. 7 gives the contour of stress (σ_z) on x-z section and distribution of rock block elements. The stress concentration is observed around rock block. Since weaker jointed elements are relatively weak, the failure initiates near the weaker jointed elements and progressively spread out to soil elements.

The average deformation versus uniaxial load is nonlinear in our simulation as shown in Fig. 8, in which the "linear result" refers to the stress versus displacement obtained by

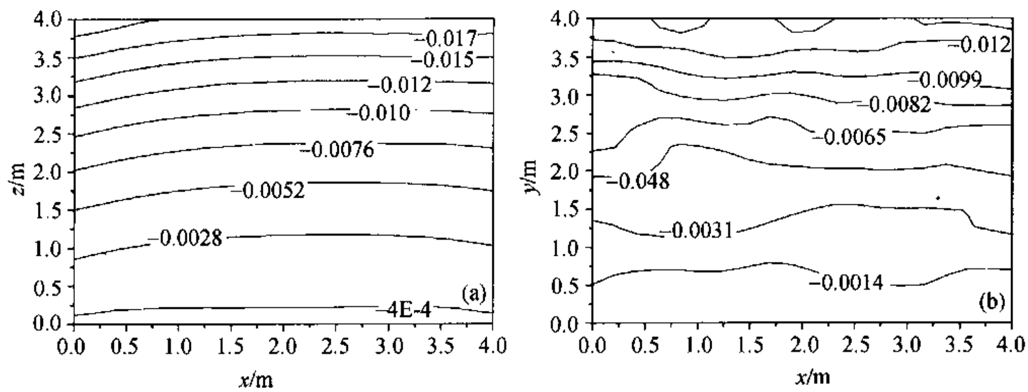

Fig. 6. Contour of displacement on x-z section for different mixture ratios. (a) 100% soil; (b) 20% rock.

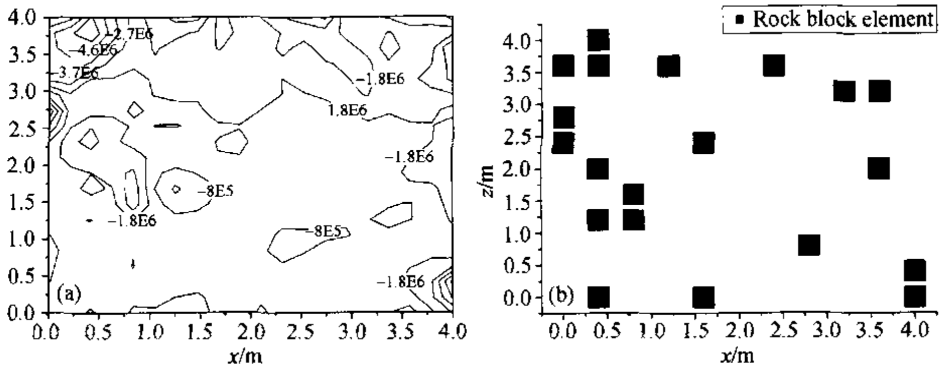

Fig. 7. Contour of stress (σ_z) on x-z section and distribution of rock block elements.

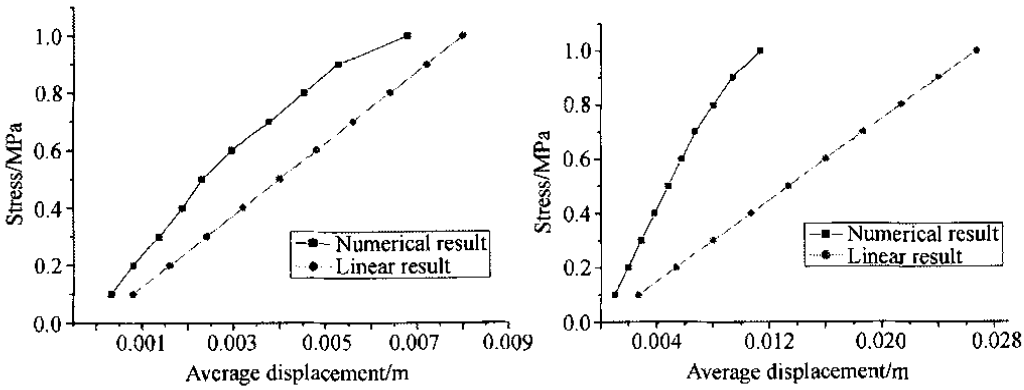

Fig. 8. Stress versus displacement curve for two mixture ratios. (a) 20% rock; (b) 80% rock.

only volume average of rock and soil components. Fig. 9 shows the effect of mixture ratio and block size of a rock on the nonlinearity of rock and soil aggregates. This nonlinearity is due to the composition of rock and soils and their interface. For a uniform rock or soil material, the relationship of deformation and load may be linear if linear elastic constitutive law is assumed. However, for rock and soil aggregates, the mechanical properties completely depend on their microstructures. Fig. 8 shows that the average

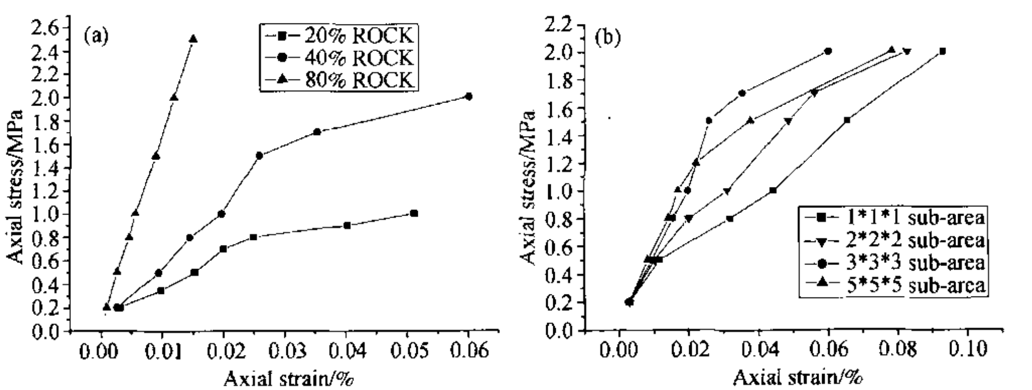

Fig. 9. Effect of geometrical parameters on stress versus strain curves. (a) Different mixture ratios; (b) different rock block sizes.

elastic modulus of rock and soil aggregates is higher than that obtained by only volume average of rock and soil components as a result of the interaction among rock and soil components[4]. Numerical simulations show that some soil elements surrounded by rock elements is not fully deformed. Therefore, for rock and soil aggregates, microstructural structure plays an important role in overall deformation and strength.

4.3 Failure simulation

The displacement and stress fields are different if failure mode is included. Local strain and stress change around failure zone, resulting in redistribution of overall strain and stress fields. Fig. 10 shows the contour of stress (σ_z) on $x = 10.5$ m cross section and distribution of rock block elements. Fig.10 (a) is the result without failure strength and Fig. 10 (b) is the result with failure strength. We can see that the stress field is redistributed when damage occurs in soil and weaker jointed elements.

This model is used to simulate the *in situ* shear test of rock and soil aggregates. A typical site is located in BAIYIAN landslide of Three Gorges Reservoir area[1]. The sample size is 90 cm×60 cm×30 cm in length, width and height, respectively. The details of test are shown in Fig. 11. From the statistically geometric parameters of rock and

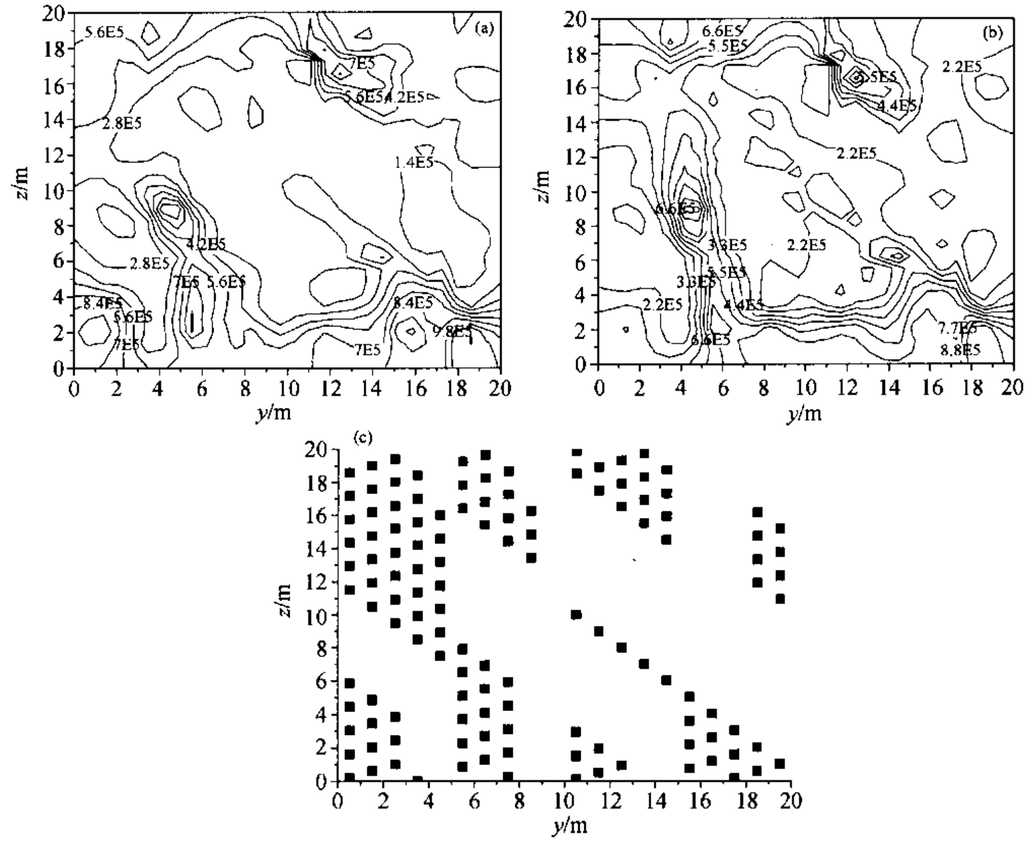

Fig. 10. Contour of stress (σ_z) on x = 10.5 m cross section and distribution of rock block elements. (a) Without considering the failure strength; (b) with the failure strength considered; (c) distribution of rock block element.

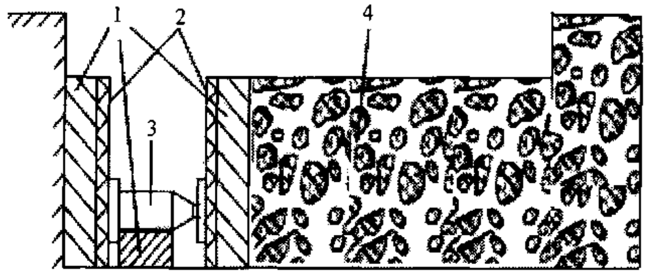

Fig. 11. Sketch of *in situ* direct shear tests on the RSA sample (from ref. [1]). 1, Crossties; 2, steel plates; 3, jacks; 4, testing sample.

soil aggregate sample, such as rock size and shape, and mixture ratio, a microstructural numerical model is constructed. The CDEM is then employed to study the mechanical response of this sample. Fig. 12 is a comparison of the fracture plane observed in numerical simulations and *in situ* test observation. The failure zones increase and are eventually concentrated along a thorough fracture plane, which is consistent with the observation in field tests, indicating that by numerical analysis based on the CDEM we can simulate failure process of rock and soil aggregates.

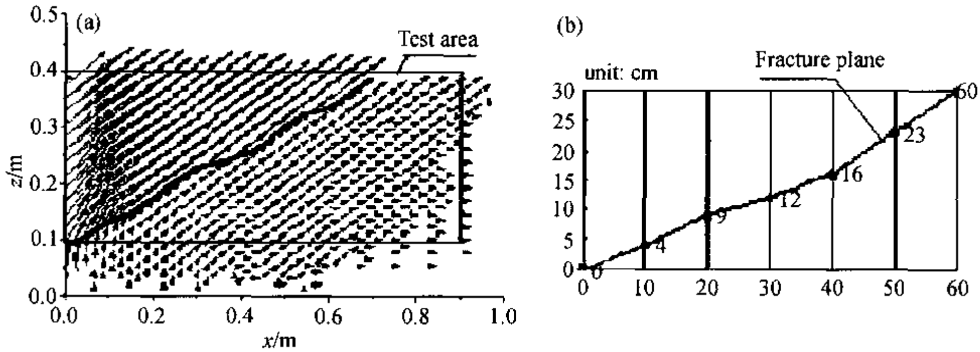

Fig. 12. Comparison of fracture plane between CDEM simulation and *in situ* observation. (a) Displacement vector and fracture plane in CDEM result; (b) fracture plane in *in situ* test.

5 Conclusions

This paper studied the stress versus strain curve and failure mode of rock and soil aggregates using continuum-based discrete element method. Numerical results are compared with *in situ* test and in good agreement with *in situ* observations. From this study, the following conclusions can be drawn:

First, the microstructure of rock and soil aggregates can be constructed by the stochastic model with mixture ratio, rock size and rock shape. The microstructure can be divided into rock element, soil element, and jointed element.

Second, the nonlinearity of RSA mainly depends on microstructure and the constitutive law of weaker joints elements. The failure is usually initialized and spread out from weaker jointed elements. The microstructure affects not only overall strength but also internal stress distribution.

Third, CDEM numerical results coincide with *in situ* test not only in nonlinear deformation but also in failure mode. Therefore, the current model applies to the mechanical behaviors of rock and soil aggregates.

Acknowledgments This study was supported by the National 973 Project (Grant No. 2002CB412703) and the important aspect project of the Chinese Academy of Science (Grant No. KJCX2_SW_L1).

References

1. Li, X., Liao, Q. L., He, J. M., *In situ* tests and a stochastic structural model of rock and soil aggregate in the Three Gorges reservoir area, Int. J. of Rock Mechanics & Mining Sciences, 2004, 41(3): 494.
2. Chen, C.G., Yao, L.K., Wang, Q., Application of three dimensional discrete element method in studies of debris-flow deposit process, J. Natural Disasters, 2003, 12(4): 55—61.
3. Zhang, B.Y., Wang, J.G., Shi, R.F., Time-dependent deformation in high concrete-faced rockfill dam and separation between concrete face slab and cushion layer, Computers and Geotechnics, 2004, 31(7): 559—573
4. Wang, J.G., Leung, C.F., Ichikawa, Y., A simplified homogenization method for mixed soils, Computers and Geotechnics, 2002, 29(6): 477—500
5. Axelrad, D R., Stochastic Mechanics of Discrete Media, Berlin-Heidelberg: Springer-Verlag, 1993.
6. Meyyer, T., Einstein H.H., Geologic stochastic modeling and connective assessment of fracture systems in the Boston area, Rock Mechanics and Rock Engineering, 2002, 35(1): 23—44.
7. Li, S.H., Zhao M.H., Wang Y.N., Rao Y., A new numerical method for DEM–block and particle model, Int. J of Rock Mechanics & Mining Sciences, 2004, 41: 436.
8. Li, S.H., Lian, Z.H., Wang, J.G., Effect of rock mass structure and block size on the slope stability—Physical modeling and discrete element simulation. Science in China, Series E, 2005, 48(Supp.): 1—17.
9. Cundall, P. A., A computer model for simulating progressive, large scale movements in blocky rock systems, Proceedings of the International Symposium Rock Fracture, ISRM, Nancy, Paper No. II-8, Vol. 1, 1971.
10. Dowding, C. H., O'Connor, K. M., Distinct element modeling and analysis of mining induced subsidence, Rock Mechanics and Rock Engineering, 1992, 25: 1—24.