NUMERICAL MODELLING OF PROGRESSIVE FAILURE IN PARTICULATE COMPOSITES LIKE SANDSTONE[①]

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ABSTRACT The beam-particle model is presented for analyzing the progressive failure of particulate composites such as sandstone and concrete. In the model, the medium is schematized as an assembly of particles which are linked through a network of brittle-breaking beam elements. The mechanical behaviour of particle elements is governed by the distinct element method and finite element method. The propagation of the cracking process in particulate composites is mimicked by removing the beam element from the mesh as soon as the stress in the beam exceeds the strength assigned to that particular beam. The new model can be utilized at a meso-scale and in different loading conditions. Two physical experiments are performed to verify the numerical results. The crack patterns and load-displacement response obtained with the proposed numerical model are in good agreement with the experimental results. Moreover, the influence of heterogeneity on crack patterns is also discussed and the correlation existing between the fracture evolution and the loads imposed on the specimen is characterized by fractal dimensions.

Key words beam-particle model particulate composites progressive failure meso-structure

1 INTRODUCTION

The numerical modelling of progressive failure in particulate composites is important in understanding the mechanisms for the generation, evolution, and interaction of stress-induced microcracks. Particulate composites like sandstone and concrete are heterogeneous or disordered materials which are very often considered as two-phase materials made of aggregates (or grains) and matrix. Density, porosity and mechanical properties are not identical at each point within a sample, which induces stress concentrations when subjected to mechanical loadings. The fracture process in particulate composites such as sandstone and concrete starts with microcracking. Microcracks are generally considered to develop from the weakest points and from the flaws or defects pre-existing among materials on various scales, mostly due to debonding between matrix and aggregates (or grains). The generated microcracks grow together and form a localized crack which leads to the failure of the whole structure. So the micro- or meso-structure of the material must be taken into account in the study of progressive failure of particulate composites like sandstone.

Most of the numerical models used for simulating progressive failure in particulate composites are macromechanical models and are based on the fictitious crack model proposed by Hillerborg *et al*[1]. These models use the fracture energy as a material property and are suitable for structural calculations. But they have difficulties in correctly representing the failure mechanisms in heterogeneous materials. The main reason for this is that the material is assumed to be homogeneous and heterogeneous meso-structure is not taken into account. Although much empirical knowledge has been gathered, there are still nu-

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merous fundamental aspects that remain unsolved. Therefore, it is important to develop a numerical model to study what may really happen in particulate composites like sandstone when taking into account their heterogeneous meso-structure in a somewhat realistic scale.

The most realistic scale used to simulate the fracture is certainly on the atomic level. Because of the existing limitations of computational capabilities, this idea is too ambitious to realize. However, with the development of fast computers, it has become possible to model the structure of the material at micro or meso level directly. The latest attempts are based on lattice techniques[2], which affirmed by RILEM in a report are very promising tools in the study of microcracking of concrete under tension[3]. In the lattice model, the material is schematized as a network of beam elements in the zone of the specimen where cracks are expected. Different material properties are assigned to the respective beam elements in matrix, aggregates (or grains) and bonds. When the maximum tensile stress in a beam is larger than its strength, this beam is supposed to break and is removed from the mesh. The crack patterns obtained with the model are in good agreement with the concrete fracture experimental observations. The main disadvantages of the model are that it is inapplicable for simulating compressive failure and the mass of the specimen under increased compressive loadings would vanish using the model, because there is no compressive failure criterion available until now. Furthermore, the lattice model can not cope with particle rotations and particle separations. Cracks induced under a compressive stress field are of the most interest because the particulate composites like sandstone are under compressive stress most of the time in practice. As a result, the application scope of the lattice model is limited to some extent.

In order to resolve the weak points of the lattice model, a meso-mechanical beam-particle model solved using an iterative scheme is proposed for simulating the progressive failure in particulate composites like sandstone. In this model, the whole medium is divided into an assembly of discrete, interacting particle elements which are linked through a network of brittle breaking beam elements. The mechanical behaviour of particle elements is modeled using the distinct element method in which particles are allowed to transmit compressive forces[4]. The new model has the combined advantages of both lattice model and distinct element model, not only suitable for simulating tensile, shearing and compressive fractures but also for simulating the postfailure behaviour, such as some fragments flying off with a high velocity.

In the following sections, we will describe the fundamentals of the beam-particle model first, and then consider the most common situation where cracking takes place in the bulk of the material under uniaxial compression as in the simulation examples. Numerical results obtained are compared with the experimental results. Moreover, the influence of heterogeneity of material on crack patterns is briefly discussed and the fractal geometry is utilized to evaluate the connectivity of cracking. The questions of what universal laws exist between the connectivity of cracking and the maximum stress that one has to apply to break the structure apart are also approached in this paper. The main objective of the investigation is to demonstrate the validity of the model, but also attention is focused on simulating the way the cracks develop and finding final crack patterns.

2 NUMERICAL MODEL

In this paper, a beam-particle model is proposed for simulating progressive failure in particulate composites like sandstone. In the model, the material is schematized as a two dimensional assembly of particle elements and nearest-neighboring particles are connected through a lattice of elastic beam elements (Fig.1). A real aggregate or grain in particulate composites may be composed of several particle elements. If a particle is created on one site where no aggregate or grain exists in reality, the particle is named as ‘matrix particle’ which functions as cementing material and transferring loadings. The rest of the particles which constitute an aggregate or grain are named as ‘reinforcing particles’. According to the types of two linked neighbouring particles, the beam elements can be classified into three types: (1) reinforcing beam, which connects two reinforcing particles; (2) matrix beam, which connects two matrix particles; and (3) bond beam, which connects a reinforcing particle and a matrix particle. Different types of beam have different elastic and strength properties. The disorder or heterogeneity of particulate composites can be easily implemented in the numerical simulation of fracture process by varying the particle sizes and beam strength, etc. Voids and other defects pre-existing among materials can be modelled by breaking beam elements in advance.

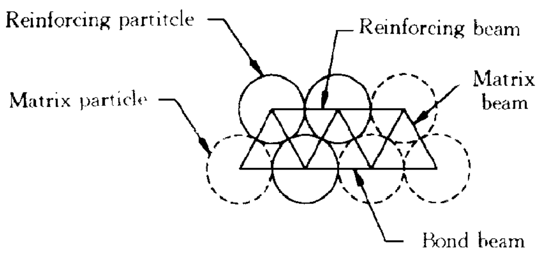

Fig.1 Schematic representation of beam-particle model

The beam-particle model uses a step-by-step approach. Due to the fact that the material structure has been modelled in detail, the model becomes inherently more simple. Detailed descriptions of the model are as follows.

2.1 Force-displacement equations for beam element

For a beam element which links two nearest-neighboring particles, there are three continuous degrees of freedom on one node i (i.e. the center of a particle): the two coordinates x_i and y_i and one flexed beam angle θ_i. The beam is to be imagined having a certain thickness and can carry axial, shear and bending forces. One defines two relative displacement variables and three material dependent constants[5]:

$$u = x_j - x_i, \quad v = y_j - y_i \tag{1}$$

$$s = EI/l, \quad \alpha = EA/l,$$

$$\beta = 14.4\, EI/(GAl^2) \tag{2}$$

where E—Young's modulus; G—shear modulus; A—area of the beam section; I—moment of inertia for flexion; l—spacing between two nodes of a beam.

Then for a horizontal beam between nodes i and j, the axial, shear and bending forces are calculated from the following equation:

$$\boldsymbol{F} = \boldsymbol{KD} \tag{3}$$

where $\boldsymbol{F} = [N_i \quad Q_i \quad M_i \quad N_j \quad Q_j \quad M_j]^T$ are the beam's node forces, $\boldsymbol{D} = \{u_i \quad v_i \quad \theta_i \quad u_j \quad v_j \quad \theta_j\}^T$ are the beam's node displacements, $\boldsymbol{K}$ is the stiffness matrix, which can be expressed as:

$$\boldsymbol{K} = \begin{bmatrix} \alpha & 0 & 0 & -\alpha & 0 & 0 \\ & B_1 & -B_2 & 0 & -B_1 & -B_2 \\ & & B_3 & 0 & B_2 & B_4 \\ & & & \alpha & 0 & 0 \\ & \text{symmetry} & & & B_1 & B_2 \\ & & & & & B_3 \end{bmatrix} \tag{4}$$

where $B_1 = \dfrac{12s}{(1+\beta)l^2}$, $B_2 = \dfrac{6s}{(1+\beta)l}$,

$B_3 = \dfrac{(4+\beta)s}{1+\beta}$, $B_4 = \dfrac{(2-\beta)s}{1+\beta}$

Similar formulas can be rewritten for vertical beams. The fracture of the particulate composites like sandstone takes place by removing the beam element as soon as its stress strength is exceeded in each load step. The stress strength σ_{cr} is derived from the following equation:

$$\sigma_{cr} = \eta N/A + \xi \max(|M_i, M_j|)/W \tag{5}$$

where N—axial or longitudinal force in the beam element; M_i and M_j—bending moments in node i and j of the beam element respectively; $A = d \times h$—cross sectional area of the beam, d—beam thickness; $h = 0.618$; l—height of the beam, $W = d \times h^2/6$; η—a scaling factor for the axial stress; ξ—a scaling factor for the bending force.

2.2 Motion laws for particle element

When beam elements are broken and removed, the particle elements freed can interact with each other based on the technique of distinct elements[6]. This technique simulates the discrete behavior of the medium by assuming that the motion of each particle may be modeled using Newtonian rigid-body mechanics with particular force-deformation and force-deformation rate contact laws. In the distinct element model, the particle element is capable of transmitting compressive loadings but cannot transmit tensile loadings. The tensile loadings can be borne by the beam elements as mentioned earlier. This distinct element model offers significant advantages for the analysis of multiple interacting, deformable and fractured bodies undergoing large displacements and rotations.

3 EXPERIMENTAL PROCEDURES AND RESULTS

If the disorder or heterogeneity of the particulate composites is taken into account, the full similarity between the physical experiments and numerical simulations is too difficult to realize. As mentioned above, the main aim of the study is to test and verify the effectiveness of the beam-particle model. For convenience, the particulate composites are supposed to be homogeneous in the following physical experiments and numerical simulation, i.e. the physical and mechanical properties of both reinforcing particle elements and matrix particle elements are all taken to be identical.

The physical experiments are conducted on specimens made of hexagonal close-packed rods of diameter 5.0 mm. The rod is carbon steel wire which has a mass density of 7.845×10^3 kg/m^3. The rod assembly is glued together by a mixture whose mixing proportions of Portland cement 425# : epoxy resin (E-44) : ethylene diamine : dibutyl phthalate: toluene are 2∶1∶0.1∶0.1∶0.1 (by mass). The specimens are removed from their moulds one day after casting and are then cured for three weeks in a laboratory condition (temperature 20 ℃, humidity 50 %).

Two different shapes of specimens are tested, namely cube and rectangular parallelepiped. The dimensions of the cube and rectangular parallelepiped are 60 mm × 60 mm × 60 mm and 60 mm × 150 mm with a thickness of 50 mm respectively. Uniaxial compressive tests are performed in a hydraulic closed-loop testing machine, under a constant rate. The loadometer (BHR-4) and the linear variable displacement transducers (LVDTs) for the axial load and displacement measurements are attached to the upper loading platen of the machine and the base of loadometer respectively. The IMP (isolated measurement pods) and IMPDAS (IMP data acquisition system) are applied to monitor and record the deformations and loads on the specimen whose both ends are not lubricated in the experiments.

The main experimental results for the compressive tests are presented in terms of crack pattern and load-displacement curve. The testing results on the cubic specimens are introduced first. Fig.2 shows the vertical cross section of the specimen that has been loaded up to failure. It can be seen that the cracks are not continuous and on whole crack pattern appears as the well known hour-glass failure mode. As a result of opening of cracks the volume of the material increases. The load-displacement response for the cubic specimen loaded up to 1.15 mm is shown in Fig.3, from which it can be seen that the specimen tends to fail in a rather brittle manner.

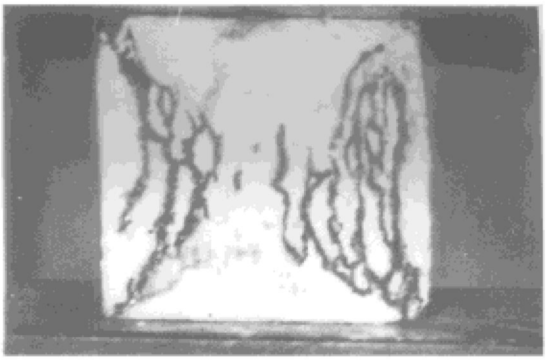

Fig.2 Crack pattern of cubic specimen loaded up to failure

Finally, Fig.4 illustrates the case of the parallelepipedal specimen described above. From the crack pattern, it is apparent that the increase of the height to width ratio of the specimen improves the chances of finding a failure mode with one dominant shear crack. This has already been observed by Van Mier[7].

4 NUMERICAL MODELLING

4.1 Comparison with experimental results

The experiments described above have been analysed using the beam-particle model under the same test conditions. All of the simulations are done under uniform and vertical boundary displacement control. The timestep used in the dynamic simulation is 1 μs. Table 1 gives the input parameters for numerical simulation, in which the mechanical properties of beam elements are determined from the corresponding macroscopic properties of the specimen according to the following empirical formulae:

$$E_b = 3.5 + 4.3\sqrt{E_c}\text{, GPa} \quad (6)$$

$$\sigma_t = 0.03 E_c^{2/3}\text{, MPa} \quad (7)$$

$$\sigma_c = 10.0\sigma_t\text{, MPa} \quad (8)$$

where E_c, E_b —elastic moduli of specimen and beam element respectively, σ_t, σ_c —tensile and compressive strength of beam element.

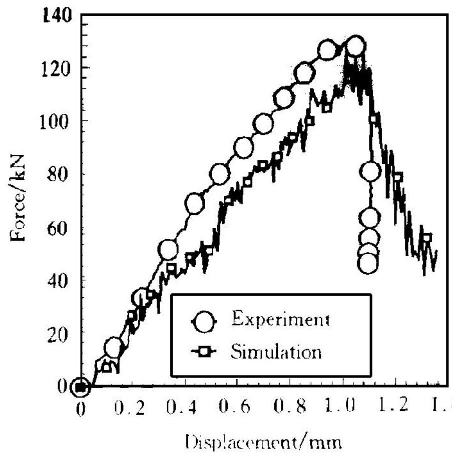

Fig.3 Experimental and simulated load-displacement curves of cubic specimen

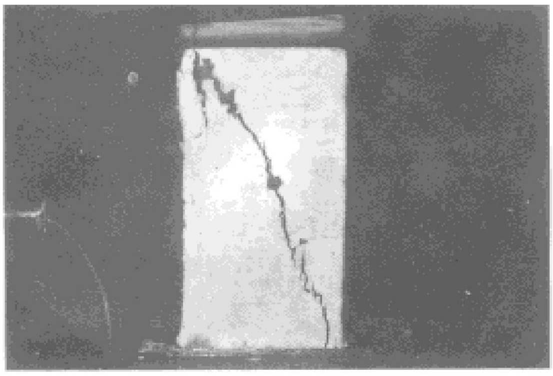

Fig.4 Crack pattern of parallelepipedal specimen loaded up to failure

Table 1 Input parameters for numerical simulation

Mechanical parameter	Value
Elastic modulus of specimen	30.0 GPa
Elastic modulus of beam	27.1 GPa
Poisson's ratio of beam	0.3
Compressive strength of beam	29.0 MPa
Tensile strength of beam	2.9 MPa
Normal and shear stiffness of particle	260 kN/mm
Friction angle	45°

The simulated progressive failure in both cubic and parallelepipedal specimens of particulate composites is shown in Figs. 5 and 6. When the simulations are compared with the experiments as shown in Figs. 2 and 4, it can be noticed that large similarities exist in the respective crack patterns, which have analogous shapes on the whole. As the height of the specimen is equal or close to its width, the well known hourglass failure mode is found, while for the specimen of a larger height to width ratio, a failure mode with one dominant shear crack is predicted. In both modes, the cracks develop intermittently in the material, so many crack and rock bridges are formed.

The load-displacement curve of the simulation with the beam-particle model on the cubic specimen is compared in Fig.3. As seen from Fig.3, the post peak behaviour simulated is less brittle than the experimental outcome. However, the level and position of the peak load can be approximately determined with the model.

4.2 Influence of heterogeneity

In order to identify the effects of heterogeneity or disorder of particulate composites like sandstone, the Young's moduli and strength of beam elements are assumed to be identically lognormal-distributed random variables. The mean values of these parameters are just the same as shown in Table 1. The uniaxial compressive tests of a specimen as shown in Fig.7(a) are taken for an example to study the influence of heterogeneity on crack pattern. When the heterogeneity of the specimen is weak, that is, the

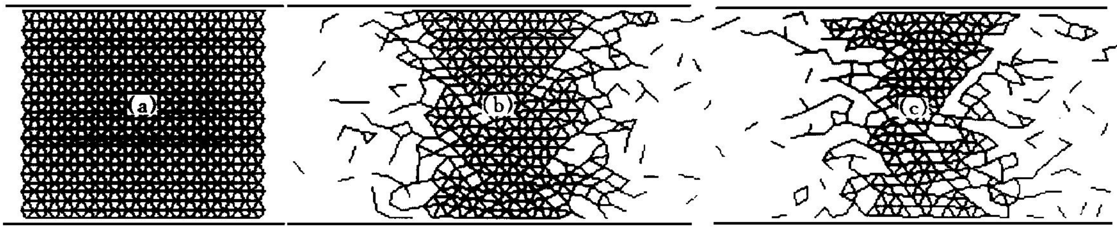

Fig.5 Crack history of cubic specimen at different stages of loading
(a) —Initial state of beam mesh; (b) —Stage 1; (c) —Stage 2

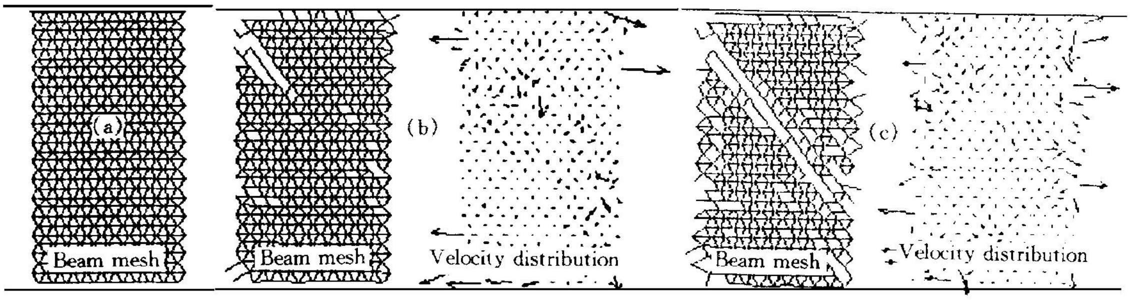

Fig.6 Crack history of parallelepipedal specimen at different stages of loading
(a) —Initial state; (b) —Stage 1; (c) —Stage 2

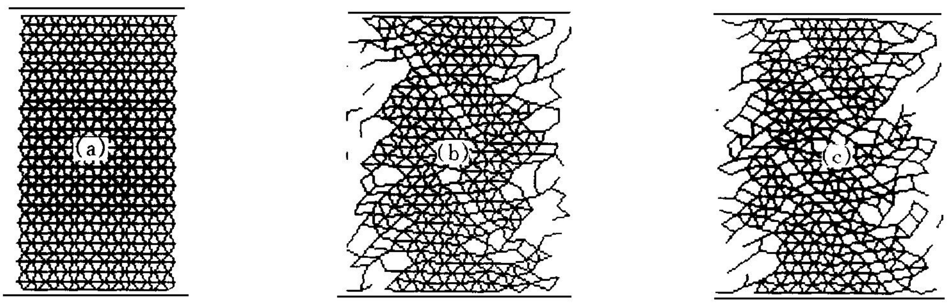

Fig.7 Influence of heterogeneity on crack patterns
(a) —Initial state of beam mesh; (b) — When heterogeneity is weak; (c) — When heterogeneity is strong

standard deviations of Young's moduli and strength of beams are 0.05 GPa and 0.01 MPa respectively, the crack pattern is shown in Fig.7 (b). And when the standard deviations of Young's moduli and strength of beams are increased to +2.5 GPa and +0.6 MPa respectively, the crack pattern is shown in Fig.7(c). From the above simulated results, it can be seen that the heterogeneity or disorder of material has much influence on the crack pattern.

4.2 Fractal characteristics of cracking

It is very important to discuss the correlation existing between the cracking evolution and the increasing compressive loading in the research on lifetime performance of particulate composites like sandstone. In this paper, this question is approached using the theory of fractal geometry[8].

There are many methods to determine the fractal dimension of crack patterns, including the divider method, box-counting method and spectral method. In this paper, the box-counting method is applied to study the fractal evolution of crack patterns under compression. From an operative point of view, this method is implemented by generating a square grid of linear dimension ε_i and determining the number $N_i(E, \varepsilon_i)$ of boxes needed to cover the entire area E. The procedure is repeated with progressively smaller box sizes. Linear regression with the bilogarithmic data ($\lg N_i$ versus $\lg \varepsilon_i$) is performed, and the fractal dimension D is obtained from the slope of the best-fitting line.

A fractal dimension field [1.4, 1.6], which characterizes the relation between the cracking connectivity and the loading level, has been found through many repeats of numerical tests. Taking the cubic specimen shown in Fig.5 as an example, just before the load exceeds the compressive strength of the specimen, the fractal dimension of the crack patterns is 1.38, less than 1.4. When the load exceeds the compressive strength of the specimen and displacement equals 1.1 mm, the fractal dimension of crack patterns is increased to 1.71, much greater than 1.6. It should be conjectured that the fractal dimensions 1.4 and 1.6 would be regarded as the critical values to evaluate the connectivity of cracking and to describe load intensity. When the fractal dimension D of crack patterns is less than 1.4, the connectivity of cracking has not been well developed and the loading imposed on the specimen can be increased. When the fractal dimension D of crack patterns is greater than 1.6, the cracks have been fully intersected and the engineering performance of the specimen has become poor.

5 CONCLUSIONS

(1) The fundamentals of inherently simple beam-particle model are explained in this paper.

(2) The crack patterns and load-displacement curves observed in the physical experiments are in good agreement with the numerical results, which have demonstrated the validity of beam-particle model for simulating the progressive failure of particulate composites.

(3) The main advantages of the model are that not only the failure modes can be correctly captured, but also the progressive dilation, especially the postfailure behaviour of specimen under different loading conditions can be simulated.

(4) Numerical examples show that the heterogeneity or disorder of material has much influence on the crack pattern.

(5) With the theory of fractal geometry successfully implanted in the model, an intrinsic link between the maximum compressive stress imposed on the specimen and the fractal dimension of crack patterns is found. Thus, the critical point when the structure of a specimen totally collapses can be predicted according to the fractal dimension.

(6) Finally, it should be admitted that the beam-particle model is still relatively coarse at the moment and systematic research work needs to be done, such as establishing more appropriate failure criterion and developing 3D beam-particle model, etc.

REFERENCES

1 Hillerborg A, Modeer M and Petersson P E. Cement and Concrete Research, 1976, 6(6): 773 - 782.

2 Herrmann H J, Hansen H and Roux S. Phys Rev, 1989, B39(1): 637 - 648.

3 Bascoul A. Materials and Structures, 1996, 29: 67 - 78.

4 Cundall P A and Strack O D L. Geotechnique, 1979, 2(1): 47 - 65.

5 Long Y Q and Bao S H. Structural Mechanics, Part 2, (in Chinese). Beijing: Higher Education Press, 1979: 298 - 303.

6 Wang Y J and Xing J B. Distinct Element Method and its Applications in Soil and Rock Mechanics, (in Chinese). Shenyang: Northeastern University Press, 1991: 60 - 89.

7 Van Mier J G M. Materials and Structures, 1986, 19: 179 - 200.

8 Xie H. Fractals in Rock Mechanics. Geomech. Research Ser. Balkema, Rotterdam/Brokfield, 1993: 58.

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