

Numerical simulation of fracture process of concrete under uniaxial compression via PFC2D

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Abstract. Simulation of cracks and cracking process is one of the difficult problems in the numerical simulation of concrete. In this paper, the discrete element method (DEM) was applied to the numerical simulation of concrete specimen under uniaxial compression and the whole process of crack generation and development were visualized. In order to simulate the three different components of aggregates, mortar and interfaces, the random aggregate model was used in the simulation. The strain-stress curves of concrete under uniaxial compression obtained from the simulation were in good agreement with experiments. These results show that the DEM can be well used to simulate the fracture process of concrete. Therefore, the study lay a foundation for the further study on the cracking mechanism of concrete members.

1. Introduction

Concrete was widely used in civil engineering, research on cracking mechanism of concrete was always a hot topic in civil engineering [1,2]. In mesoscopic level, concrete was often viewed as a heterogeneous composite materials composed of coarse aggregate, cement mortar and interfacial zones between the two ingredients [3]. Wittmann [4] thought the mechanical properties of concrete under a certain scale could be explained by a lower scale structure of the concrete, therefore, study of concrete within meso-scale was helpful to deep understand the macroscopic failure mechanism of concrete and its mechanical characteristics.

Much experimental researches has been conducted on fracture mechanism at the meso-scale in the past [5,6]. In such research, fracture propagation from the interface between mortar and aggregate to the mortar part was observed in compression experiment and the effect of the aggregate on nonlinearity of the macroscopic stress-strain curve of concrete and the failure of concrete are mentioned. However, experiment study was time-consuming and inefficient, therefore, in recent years, as the rapid development of computing power and numerical method, research at the meso-level from the numerical point of view has begun but has not been conducted far enough yet.

There are many approaches to be used to model the meso-structure and the fracture process of concrete, but most of them fail to describe the behavior of discontinuous zones [7]. Previous numerical simulation work using continuum analysis could well indicate the stress distribution and got a relatively good stress-strain curve. However, fractures cannot be explicitly represented using the continuum approach. Compared with the finite element method, the discrete element method (DEM) has numerous advantages for crack formation [8].

Particle flow code (PFC) provided an embodiment of the discrete element method for the analysis of concrete-mechanics problems. The PFC method was proposed by Cundall [9] in 1979, it use Newton's second law to calculate the motion of particles, so the large deformation of material can be easily capture. Through applying bonds between particles, PFC can simulate the process of material transformation from continuum to dispersion under load. For its unique advantages in simulating



granular materials, it has been widely used in geotechnical engineering [10,11] and the failure process of material, especially rocklike materials, within the meso-level.

In the present work, a random aggregate model of concrete was created first, then the fracture process was simulated by the PFC2d based on the random aggregate model, finally, the numerical simulation results were compared with the experimental results, and the simulation results were discussed.

2. PFC method

The research object is discretized into many small rigid disks with quality in PFC2d, the interaction between discs is expressed by the contact model, which can be linear or nonlinear with their corresponding failure criteria. The movement rules are very simple, so particles can be rotated or translated arbitrarily only to obey the Newton's laws of motion [12]. In the PFC model, the constitutive relations of materials are not needed, and all of the macroscopic mechanical properties can only be expressed by defining the interactions between particles. Therefore, the contact type and its parameters selection are the key to success of PFC numerical simulation. There are some built-in contact models in PFC, these models can meet needs of most analysis. Linear Parallel Bond Model is a built-in contact model which was frequently adopted in the simulation of concrete and was verified reliable. Therefore, the LPBM was chosen at the present work to simulate the contact inner concrete.

2.1. Linear Parallel Bond Model

A parallel bond provides the mechanical behavior of a finite-sized piece of cement-like material deposited between the two contacting pieces (similar to the epoxy cementing the glass beads shown in figure 1). The parallel-bond component acts in parallel with the linear component and establishes an elastic interaction between the pieces. The existence of a parallel bond does not preclude the possibility of slip. Parallel bonds can transmit both force and moment between the pieces.

A parallel bond can be envisioned as a set of elastic springs with constant normal and shear stiffnesses, uniformly distributed over a rectangular cross-section lying on the contact plane and centered at the contact point. These springs act in parallel with the springs of the linear component. Relative motion at the contact, occurring after the parallel bond has been created, causes a force and moment to develop within the bond material. This force and moment act on the two contacting pieces and can be related to maximum normal and shear stresses acting within the bond material at the bond periphery. If either of these maximum stresses exceeds its corresponding bond strength, the parallel bond breaks, and the bond material is removed from the model along with its accompanying force, moment, and stiffness.

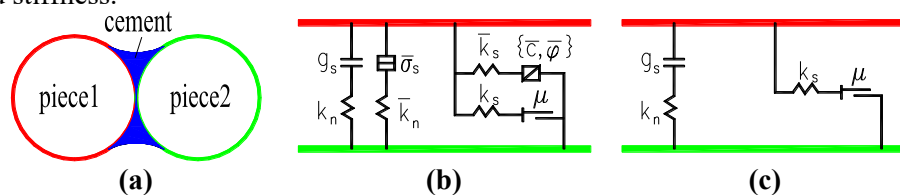


Figure 1. Linear parallel bond model: (a) diagram of LPBM; (b) mechanical model of bonded state; (c) mechanical model of unbonded state

The force-displacement law for the linear parallel bond model updates the contact force F_c and moment M_c :

$$F_c = F^l + F^d + \bar{F}; \quad M_c = \bar{M} \quad (1)$$

Where F_l is the linear force, F_d is the dashpot force, \bar{F} is the parallel-bond force, and \bar{M} is the parallel-bond moment.

2.2. The method of modelling

According to the Walraven formula, the size and quantity of coarse aggregate on the two-dimensional specimen were calculated by MATLAB based on the Fuller gradation curve [13]. Then the polygonal

aggregates were randomly generated according to the size and quantity and so the geometry of random aggregate model was accomplished. In this study, the size of specimen is 100mm×100mm and the coarse aggregate fraction was 0.25, 0.3 and 0.35 respectively, the maximum and the minimum radius of the coarse aggregate was 25mm and 10mm, respectively.

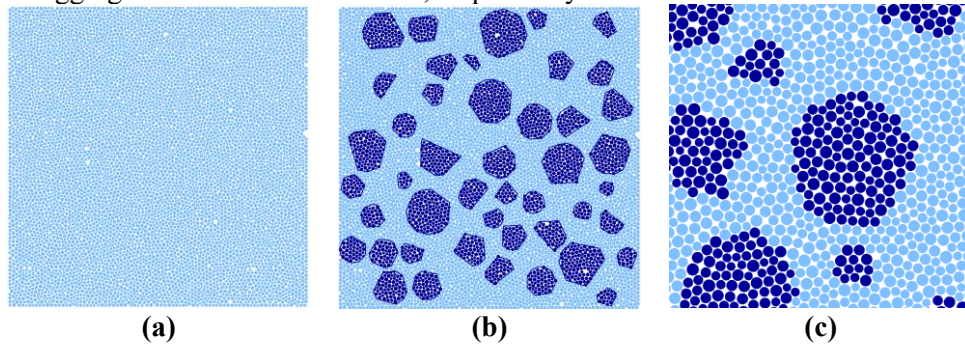


Figure 2. Numerical model: (a) The initial fine particle system; (b) The particle system with coarse aggregate; (c) The details view of model. The dark blue particles denote coarse aggregate, while the light blue particles denote cement.

Particles with radius 0.5~1mm were randomly generated within a rectangular region without gravity, as illustrated in figure 2. The initial generated particles may overlap and produce overlarge contact force in the initial particle system. The velocity of particles accelerated by the overlarge contact force were set to zero per 10 cycles before 2000 cycles to prevent the particles from escaping the rectangular region. To quickly reach the equilibrium state, the initial system was frictionless. In order to further reduce the kinetic energy of the initial particle system, the mass-scale method was adopted to solve until the ratio of the mean static unbalanced force to the mean static contact force was less than 10^{-5} . Next, the geometry of the random aggregate model created in the previous step was imported to divide the particles into coarse particle group representing coarse aggregate and fine particle group representing mortar (see also figure 2). Based on the groups, the contact can be categorized into three types: coarse particle to coarse particle (CC), fine particle to fine particle (FF) and coarse particle to fine particle (CF).

Table 1. Input meso-parameters in the DEM simulations.

Meso-parameters [Units]	CC	FF	CF
Effective modulus, E , [MPa]	1.21×10^{10}	1.21×10^9	1.21×10^9
Normal-to-shear stiffness ratio, κ , [-]	1.0	1.0	1.0
Friction coefficient, μ , [-]	0.3	0.3	0.3
Tensile strength, σ , [MPa]	1.31×10^8	1.31×10^7	2.62×10^6
Cohesion, c , [MPa]	2.64×10^8	2.64×10^7	5.28×10^6
Friction angle, θ , [Degree]	50	30	10

Eventually, the initial contact type was changed to bond contact and the corresponding parameter values were assigned. It was well knew that the properties of coarse aggregate, cement mortar and interfacial zones between the two ingredients are different, the contacts of CC, FF and CF can used to express this deference by assigning different property values to different contact types. The parameters of the linear parallel bond contact adopted in this study are listed in table1. Generally, the particles and the bonds between the particles respectively have effective modulus and normal-to-shear stiffness ratio. However, in most cases the values of the two could set equal so as to simplify the analysis. Furthermore, the effective modulus and the normal-to-shear stiffness ratio should be converted firstly to normal stiffness (k_n) and shear stiffness (k_s) as follows,

$$k_n = \frac{E}{L}; \quad k_s = \frac{k_n}{k^*}; \quad \text{with } L = \begin{cases} R^{(1)} + R^{(2)}, & \text{ball-ball} \\ R^{(1)}, & \text{ball-facet} \end{cases} \quad (2)$$

Where $R^{(1)}$ and $R^{(2)}$ denote the radius of the two contact particles.

2.3. Macroscopic Variable Definitions

Before the beginning of numerical experiment, the wall on both sides of the specimen were removed. The force was load to the specimen by applying a constant velocity to the top and bottom walls, for quasi-static loading, the velocity applied to the wall was limited less than $100\mu\text{e}$ per seconds. The axis strain (i.e., ε_1) is estimated from the boundary movements, which can be defined as follows:

$$\varepsilon_1 = \frac{h_0 - h}{h_0} \quad (3)$$

Where h_0 is the initial height and h is the height at current state. The macro-scale axis stress for the meso-scale quantities of contact forces and contact vectors is as follows:

$$\sigma_1 = \frac{1}{2B} \left(\sum_{c \in N_t} f_v^c - \sum_{c \in N_b} f_v^c \right) \quad (4)$$

Where f_v^c is the vertical component of the contact force at contact c within the assembly, B is the width of the assembly, N_t is the total number contacts of particles to top wall and N_b is the total number contacts of particles to bottom wall.

3. Results and discussion

The coarse aggregate fraction is an important parameter of the concrete. Therefore, three random aggregate concrete models with different coarse aggregate fractions (0.2, 0.25 and 0.3) were studied in the present work. Loading process was realized by fish language, through the fish programming language, the stress-strain curve can be monitored in real time. When the stress drops to twenty percent of the peak stress, the numerical test stops. The transmission path of contact force and the visualization of cracking are the most important advantages of the PFC method, during the simulation, the visualization of the force chain and the cracking process are shown in figure 4. By formulation 3~4, the macroscopic stress-strain curve can be draw as figure 3.

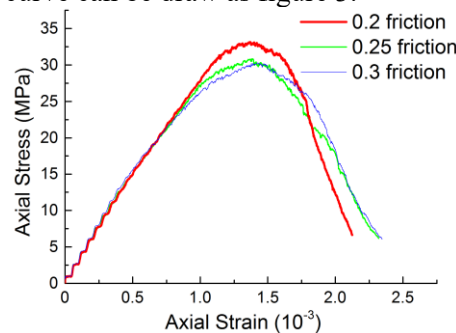


Figure 3. Stress-strain curves of different coarse aggregate fraction

As shown in figure 4, at the beginning of the test, the compressive stress level was low and it could be seen that the force chain distribution was uniform, fine and dense. Due to the low strength of interfaces, there were some internal micro cracks on the coarse aggregate surface, however, no macroscopic cracks were visible on the specimen surface. The stress-strain curve was linear, indicating that the specimen was in the state of elastic stress. With the increase of the pressure, the micro cracks on the coarse aggregate surface slowly expanded to the interior of the mortar, then visible cracks begun to form. As the pressure increased, these cracks continued to develop deep into the mortar, finally, the micro cracks in some positions connected with each other, macroscopic cracks

were clearly visible. In this stage, the force chain of cracked place disappeared while the uncracked place became stronger, the force chain distribution became not uniform and concentrated to some place. When the macro cracks appeared, the stiffness of the specimen degenerated and the stress state entered the elastic-plastic stage. With the further increase of the pressure, the stress-strain curve arrived the peak and then decreased sharply, cracks developed rapidly and the existing cracks fast connected with each other. Finally, the specimen was divided into small blocks with coarse aggregate as the core, only a few of thick force chain remain, the specimen was completely crushed and the test was over.

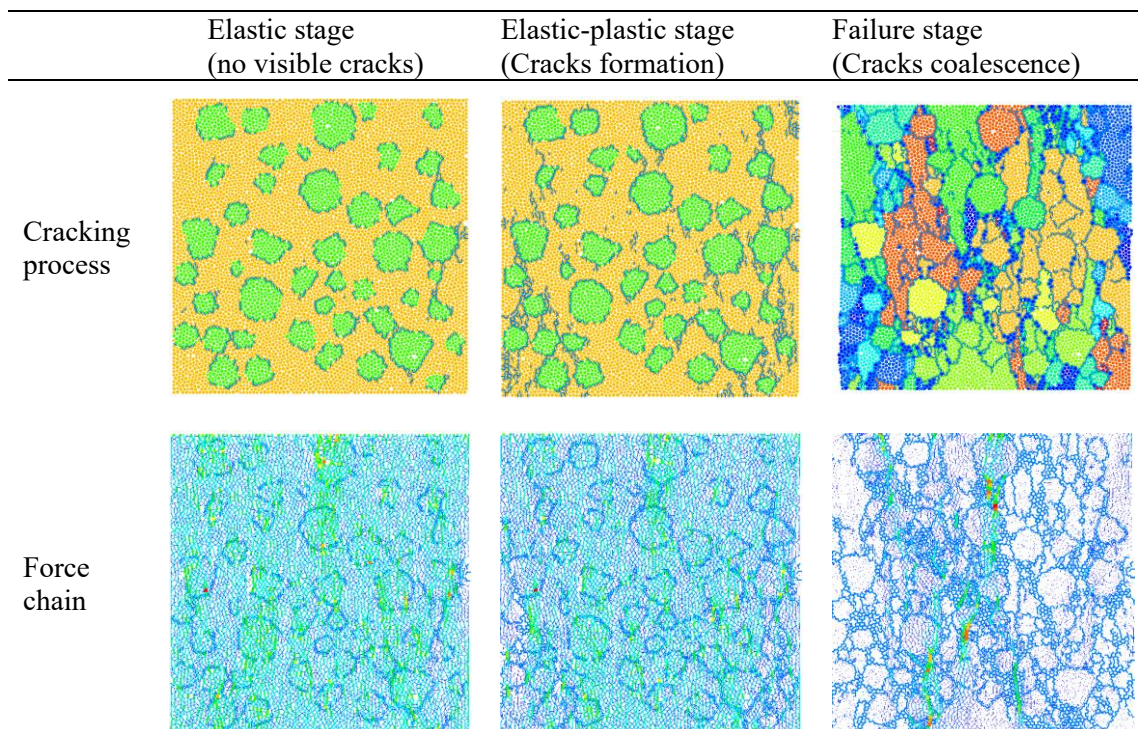


Figure 4. Visualization of fracture process

4. Conclusion

The PFC method was studied in this work to simulate the fracture process of concrete specimen under compression. The whole process of crack generation and development could clearly observed through the simulation, this is an important advantage of PFC method compared to physical experiment. In order to simulate the concrete specimens of high fidelity, the random aggregate model was used to simulate the specimen geometry, the results show that the method can accurately simulate the mechanical properties of concrete with coarse aggregates, mortar and interfaces and the stress-strain curves obtained from the simulation are in good agreement with physical experiments.

Application of PFC method to concrete is a new way to study the cracking mechanism of concrete structures by numerical simulation. The study on the cracking mechanism of concrete members by using PFC method will be the focus of the next step.

References

- [1] Ooi, E. T., Natarajan, S., Song, C., & Ooi, E. H. (2016). Crack propagation modelling in concrete using the scaled boundary finite element method with hybrid polygon–quadtree meshes. *International Journal of Fracture*, 1-23.
- [2] Schlangen, H. E. J. G. (1993). Experimental and numerical analysis of fracture processes in concrete. *Delft University of Technology*, 38.
- [3] Nilsen, A. U., & Monteiro, P. J. (1993). Concrete: a three phase material. *Cement and Concrete*

- Research*, 23(1), 147-151.
- [4] Wittmann, F. H. (1983). Structure of concrete with respect to crack formation. *Fracture mechanics of concrete*, 43(5), 6.
 - [5] Kamalibernard, S., Keinde, D., & Bernard, F. (2014). Effect of aggregate type on the concrete matrix/aggregates interface and its influence on the overall mechanical behavior. a numerical study. *Key Engineering Materials*, 617, 14-17.
 - [6] Gu, X., Hong, L., Wang, Z., & Lin, F. (2013). Experimental study and application of mechanical properties for the interface between cobblestone aggregate and mortar in concrete. *Construction and Building Materials*, 46, 156-166.
 - [7] Camborde, F., Mariotti, C., & Donzé, F. V. (2000). Numerical study of rock and concrete behaviour by discrete element modelling. *Computers and geotechnics*, 27(4), 225-247.
 - [8] Wang, Z., Lin, F., & Gu, X. (2008). Numerical simulation of failure process of concrete under compression based on mesoscopic discrete element model. *Tsinghua Science & Technology*, 13, 19-25.
 - [9] Cundall, P. A., & Hart, R. D. (1992). Numerical modelling of discontinua. *Engineering computations*, 9(2), 101-113.
 - [10] Potyondy, D. O., & Cundall, P. A. (2004). A bonded-particle model for rock. *International journal of rock mechanics and mining sciences*, 41(8), 1329-1364.
 - [11] Zhou, S., Zhu, H., Yan, Z., Ju, J. W., & Zhang, L. (2016). A micromechanical study of the breakage mechanism of microcapsules in concrete using PFC2D. *Construction and Building Materials*, 115, 452-463.
 - [12] Itasca. User's manual for PFC2D version PFC5.0. Minneapolis. USA: Itasca consulting Group, Inc; 2014.
 - [13] Wriggers, P., & Moftah, S. O. (2006). Mesoscale models for concrete: Homogenisation and damage behaviour. *Finite elements in analysis and design*, 42(7), 623-636.