The Modelling of Compressive Strength of Concrete on Discrete Element Method

Faqih Ma’arif1, Zhengguo Gao1, Feng Li1
Dept. of Transportation and Civil Engineering, Beihang University, Beijing 100083
Email: faqihmaarif07@buaa.edu.cn, gaozg@buaa.edu.cn, lifeng98@buaa.edu.cn

Abstract. This paper investigates the compressive strength of concrete in a 3-dimensional contact problem using the Discrete Element Method (DEM). This method was chosen because it can simulate the development of a single fracture up to massive fragmentation, including cracks pattern and coalition. The experimental test consisted of four cubes with 150x150x150 mm in dimensions, the constant of axial load applied to each specimen of 0.05Po up to 0.70Po. The data analysis has been carried out in Discrete Element and opensource three-dimensional code (YADE). The spherical Particles were used to the material models of concrete cubes. The pulse velocity parameter proposed to determine the behavior of the material during loading. The DEM and pulse velocity results illustrate the conformity of the relationship between stress and strain, deformation characteristics, and compressive strength of concrete.

Keywords: concrete, compressive strength, DEM, pulse velocity.

1. Introduction
The development of concrete technology is in line with the invention of solutions using modern computing techniques. The phenomenon of cracking, fracture at the macro and micro scale becomes an interesting discussion by researchers [1], [2], [3]. Various models have been developed to improve performance and concrete weaknesses.

Currently, one of the particle modeling approaches that can be used is the Discrete Element Method (DEM). DEM considers that concrete consists of a variety of particles that interact with each other (soft and hard particles). DEM analysis can model fractures in real conditions compared to the Finite Element Method (FEM). In this paper, to evolve a concept of the concrete failure mechanism on an aggregate scale in the level of macroscopic, the discrete element (DEM) method is used. In DEM, the mechanical response of a material arranges by interactions on contact round the element and particles. Likewise, the boundaries conscientious for the complexity of the phenomena that occur in this material. To reproduce concrete behavior, the YADE 3D round disk element model was used.

DEM testing for concrete in YADE has been carried out by various researchers [2], [3], [4], [5], [6], whose results indicate a level of compatibility with experimental tests. In its development, to describe the internal conditions of particles used X-Ray ICT Images methods [18], 3D laser scanning, tomography, or thin section analysis [26], but the implementation of this test is too expensive.

The proposed method to describe concrete particles’ internal condition is using Ultrasonic Pulse Velocity (UPV). This method can monitor the realtime conditions referred to as the pulse velocity (v). UPV has been used to predict the compressive strength of concrete, estimate cracks in concrete, and measure concrete homogeneity [16]. Besides, DEM results are compared with experimental laboratory and non-destructive tests. The experimental test were analyzed using YADE approach. Hereafter, new
findings show the part of DEM in supporting NDT tests using ultrasonic pulse velocity. Finally, the method developed by referring to the interaction of aggregate granules using NDT is one practical solution and can be implemented in a short and precise time. The use of uniform granules in the 3D analysis also simplifies the analysis in this paper.

2. Discrete Element Method

DEM in concrete proceeds to be generated by researchers [7], [12], [13], [14], [15], to get satisfying results. The study of the micro or macroevolution of structures in concrete (stress and strain localization) by modeling 3D on uniform granules was carried out using YADE [17], [18], [3]. In YADE, a soft-particle approach is used, which allows the deformation of the particles. There are two essential parts in YADE, including the strength of interaction, which will be calculated when the discrete elements have penetrated each other. Newton's second law is applied to calculate each particle. The acceleration results have been generated to get the latest position, and these steps will repeat until the simulation finish. Hereafter, normal and tangential vectors are the decomposition of the interaction force vector (F), representing two discrete elements of the ball in contact. The elastic law with cohesion is applied to model the normal forces on the spheres.

\[ \bar{F}_n = K_n U \bar{N} \]  
\[ \bar{F}_s = \bar{F}_{s,prev} + K_s \Delta \bar{X}_s \]

Where \( \bar{F}_n \) is the normal force vector, \( K_n \) is the normal stiffness, \( U \) is the overlap between the spheres, \( \bar{N} \) is the normal vector at the contact point, \( \bar{F}_{s,prev} \) is the tangential force of the previous iteration, \( K_s \) is tangential stiffness, and \( \Delta \bar{X}_s \) is the incremental tangential displacement value. Modulus of contact grains (\( E_c \)) and grain radius of \( R_A \) and \( R_B \) are used to determine the value of normal stiffness (\( K_n \)). Whereas the Modulus of elasticity (\( E_c \)), Poisson ratio (\( \nu_c \)), and \( R_A \) and \( R_B \) grain radii are used to calculate the tangential stiffness (\( K_s \)). \( K_n \) and \( K_s \) are calculated by the equation [17] (3).

\[ K_n = E_c \frac{2R_A R_B}{R_A + R_B} \quad \text{and} \quad K_s = \nu_c E_c \frac{2R_A R_B}{R_A + R_B} \]

If it is assumed \( R_A = R_B = R \), then the normal and tangential stiffness parameters for \( K_n = E_c R \) and \( K_s = \nu_c E_c R \), respectively. \( \nu_c \) is determined by the comparison between tangential and normal stiffness (\( \nu_c = K_s / K_n \)). For tangential and normal contact force (\( F_s \) and \( F_n \)) should satisfy the requirement of the Mohr-Columb equation for cohesive-friction in the equation (4).

\[ ||\bar{F}_s|| - \bar{F}_s^{\text{max}} ||\bar{F}_n|| x \tan \mu \leq 0 \quad \text{(before contact breakage)} \]
\[ ||\bar{F}_s|| - ||\bar{F}_n|| x \tan \mu \leq 0, \quad \text{(after contact breakage)} \]

\( F_s^{\text{max}} \) is a cohesive force between spheres, \( \mu \) is the friction angle that occurs between particles. If \( F_n^{\text{min}} \) is reached, the contact will be interrupted. The next procedure for cohesion between balls is not taken into analysis when contact appears for second time.

When the critical threshold has reached the maximum limit, the grains' strength disappears, and the particles' cracks will develop. In [17], it is explained the fragmented motion, which consists of a spring-mass with cohesion with considered to be similar to a rigid body movement. Researchers [22] reported that cohesive and tensile forces are assumed a functions of cohesive stress (\( C \)), normal stress (\( T \)), and sphere (\( R \)). In this step, the shear stress maximum is zero. \( F_s^{\text{max}} \) is calculated by the equation [22] (5).

\[ F_s^{\text{max}} = C x R^2 \quad \text{and} \quad F_n^{\text{min}} = T x R^2 \]

The smaller values of \( C, T, \) and \( R \) are assumed for the two contacts. The non-viscous damping is applied to control excessive kinetic energy in the DEM system. The parameters refer to classical theory [23] and determined based on equation (6).
\[ \vec{F}^k_{\text{damped}} = \vec{F}^k - \alpha \cdot \text{sgn}(\vec{u}^k) \cdot |\vec{F}^k| \]  

(6)

Which \( \vec{F}^k \) and \( \vec{u}^k \) is the kth component of residual strength and translational speed. The \( \text{sgn}(\cdot) \) is the value to return the speed component (k). The k values of the 3D vector can be applied in x, y, and z-direction. The parameter of \( E_c, \nu_c, \mu, F_n, F_s \) are determined based on the results of laboratory min max experiments. The value of the radius (R), mass density (\( \rho \)), damping (\( \alpha \)), and other standards are determined based on fundamental and relevant references.

2.1. UPV Test

Ultrasonic pulse velocity is one of the non-destructive test methods. The test is carried out by scattering ultra waves from the transducer (T) to the receiver (R). There are several techniques in this test, including direct, indirect, and semi-direct methods. This study was conducted using the direct method.

![Fig. 1. Schematic of experimental testing.](image)

The direct method was chosen because it has a high level of accuracy [16]. Figure 1 shows that the implementation of the direct method in five-point. There are four concrete specimens consist of Reference Cube (C_R), Cube 1 (C_B01), Cube 2 (C_B02), and Cube 3 (C_B03), with 150x150x150mm in dimensions. Reference cube (CR) is performed to find the maximum load value (P). C_B01, C_B02, C_B03 specimens are UPV tests when subjected to axial loads. Axial loads were applied from 0.05P_0, 0.1P_0, 0.15P_0, 0.7P_0 up to collapse. UPV testing is carried out on each load by stopping the test machine. In this case, there are five tests of wave spread, referring to Figure 1. The result of UPV test is travel time (TT). Further, the value is converted to velocity (v) according to equation (7).

![Fig. 2. Schematic of Pulse Velocity Apparatus using direct method [20].](image)

The value of pulse velocity is determined by equation (7).

\[ v = \frac{L}{T} \]  

(7)

where \( v \) is the velocity (m/s), \( L \) is the distance between the transducer and receiver (m), and \( T \) is the travel time (s).
3. Results And Discussion

3.1. Discrete Element Method

The simulation with YADE was created by 3D modeling. The uniform spherical particles carried out to simplify calculations without reducing the material characteristics of the experimental test. The matrix between aggregate and cement was express according to the concrete model \([\text{Ip2_CpmMat_CpmMat_CpmPhys()}]\) with constitutive law by [17]. In DEM analysis, the number of microporosity in concrete is uncounted as macroporosity. The modulus of elasticity (\(E_c\)), Poisson's ratio (\(\nu_c\)), mass density (\(\rho\)), and interparticle friction angle (\(\mu\)) of the material are determined \(E_c = 15\text{GPa}\) and \(\nu_c = 0.2\), \(\rho = 2,500\text{ kg/m}^3\) and \(\mu = 30^\circ\), respectively.

The particle packing slightly affects the stress-strain yield (around 5%) using the same grain size of distribution curve [24]. The loading rate in a quasi-static test determined at (0.25±0.05MPa/s) following the standards by [25]. Besides, for experiment test was used the rate of load (0.35MPa/s) by [26]. The number of particles applied to the concrete cube specimen is 1000 spheres. The uniform particle packaging uses a 3mm diameter, which is selected after several considerations, including analysis times and energy consumes. The iteration period is used per 100 steps. The iteration is terminated if the test collapses and reaches more than 10,000 of computation.

On the other hand, the simulation variations are carried out by modifying the speed control according to the procedure [26]. The loading rate effects to the compressive strength of concrete, it is around 5-10%. The experimental test results obtained a maximum load of 810kg with \(f'_c = 36\text{MPa}\). Meanwhile, the DEM analysis results with the YADE program show that the compressive strength is 34.32MPa. The difference of \(f'_c\) between experiments and DEM is 4.89%, which means that the DEM approach is prescribed for concrete analysis procedures in the macro- material particle model as [1].

3.2. UPV test

Ultrasonic pulse velocity testing was carried out at five points. The test results are an interpretation of the internal interaction of concrete particles.

![Fig. 3. UPV test results.](image_url)

Figure 3 reported the pulse velocity of particles in concrete for each specimen. The wave propagation decrease when the axial load increases. A smooth crack precedes the initial damage on 30% of axial force. Fine cracks preceded initial damage in 30% of the axial force and detected through travel time.

Further, cracks will occur in the same region and extend to spread. Wave dispersion is affected by crack width that occurs between the grains. The void between particles will cause the pulse velocity to decrease. In concrete tests, the density affected the values and quality. Some parameters that cause travel time differences are aggregate grains, cement water factor, voids, compressive strength, and density [16].

The coefficient of variance is one of the parameters that indicate the test satisfies the quality [16]
with values of less than 10\% (Figure 3). The linear curve illustrates the unique characteristics of concrete, even though the analysis is represented as homogeneous materials.

Concrete consisting of 4-phase materials [8], [9], [10], [11] does not consider in this analysis. In its development, this simplification caused a difference between study and experiment. Generally, experimental test results indicate that the concrete quality satisfies the grading standard's pulse velocity criteria by [21].

3.3. Crack pattern

Cracks that occur in concrete because it exceeds the limit of tensile strength. This initiation starts with fine cracks, which are initially <1mm. The crack continues to expand until the release of bonds between the aggregate particles. When the load reaches its ultimate limit, the concrete surface will be peeled off in the form of spalling.

The behavior of the material during compression shows the normal force's direction parallel to the vertical axis. In contrast, the tensile strength is identified with the horizontal direction perpendicular to the deformation plane; and the cracked area has been a reduction in contact. It is in line with the decrease in bonds. Further, cracks will develop when one of the main bonds is broken, which causes the development of the damage round between particles.

![Illustration of contact particle damage in DEM.](image)

Figure 4 shows that spheres are connected to discrete elements, and cracks occur between spheres in a vertical direction Figure 4(a). The contact between the particles is degraded due to fracture and internal material dilatation. Cracks cause particles of contacts to decrease during compression and tension in Figure 4 (b). The damage can be detected by UPV testing. The breaking of bonds due to cracking is detected by wave dispersion. The spread of cracks will reduce the intensity of the waves that spread to particles and bonds. In this condition, an increase of axial force will cause a higher intensity of stresses and crack.

Nevertheless, the material's behavior, which is not uniform during compression, causes vertical directional stress and horizontal strain. It contributed to an increase in the pulse velocity by 10\%. Thus, the use of spherical particles coincides with the DEM rules in simplifying the analysis. Lastly, the combination of DEM and UPV methods can satisfactorily describe the characteristics of macroscopic material. Even though some parameters are not fully involved in this analysis, the deficiency can be accomplished by UPV testing.

4. Conclusion

DEM modeling in a concrete cube using uniform particles in YADE can describe of damage pattern that is quite similar to an experimental test. The UPV method's reliability is one of the solutions to solve the problems that can be adopted as a comparison in detecting the behavior of concrete. Combining the proposed method by the author can simulate the compressive strength behavior of concrete specimens under axial static loading.
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