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Discrete Element Method Approach to Simulate Cracks in Four-Point Flexural Test

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ABSTRACT

Concrete is a material that is widely used in construction. Concrete research efforts are ongoing and through a series of experimental tests. On the other hand, experimental tests require a lot of money, take a long time, and create waste. Several studies have revealed that numerical testing can accurately test concrete to fractures. However, modeling for the four-point load flexure test pattern is still not widely discussed. This study aimed to model the four-point flexural test of concrete using the discrete element method (DEM) approach. Sieve gradation was performed to determine particle size, and flexure testing was performed to calibrate the DEM model. DEM flexure testing was made using Yet Another Dynamic Engine (YADE) software with ASTM D6272 reference and beam dimensions 105 x 105 x 535 mm. The cohesive contact model with spherical particles is used, and the algorithm developed modifies the faceted sphere of interaction. The study results revealed that DEM can simulate crack behavior in flexural testing of unreinforced concrete. The DEM results show only a 2.13% difference in the experimental results of the flexural strength test. Meanwhile, crack behavior can be observed directly in the DEM simulation. The results of this study can be used to predict the failure pattern of the flexural test structure and to design the right proportion of the mixture to match the desired flexural strength. So that material efficiency and concrete flexure testing time can be achieved.

1. Introduction

Concrete is widely used in construction, with production reaching 5.3 billion cubic meters annually worldwide [1]. Concrete demand is expected to increase substantially to close to 18 billion tons per year by 2050 [2]. With this high demand, concrete has become the object of much research. Several concrete innovations have been developed, such as fiber concrete [3], ultra-high performance concrete (UHPC) [4], self-compacting concrete (SCC) [5], and self-healing concrete [6]. However, it must undergo a series of laboratory tests to develop this technology.

Conducting experiments to test concrete incurs significant expenses [7]. In addition, concrete testing takes a long time because the concrete must go through a hardening process first [8]. Also, experimental testing of concrete requires sophisticated and expensive equipment. The average experimental testing of concrete is mostly destructive [9]. So much concrete waste is generated from the test [10]. Concrete unused and scattered waste only becomes garbage that piles up and can contaminate the soil because of its cement content [11]. Therefore, numerical testing is one of the solutions for conducting concrete testing [12].

Several studies have revealed that numerical testing can simulate concrete testing with fairly good accuracy [13]. One of the tests using the finite element method (FEM) approach can model the flexural loading on geopolymer concrete beams [14]. However, the discrete element method (DEM) approach is used in modeling concrete cracks because the continuum-based analysis cannot reveal events that occur at the micro-scale until the fracture boundary is reached. In addition, the DEM method can simulate mixing fresh concrete by considering the effect of adding water and changes in moisture distribution and simulating the flow process in SCC concrete [15], [16]. In addition, DEM can reveal the compression behavior of uniaxial concrete in 2D and 3D up to the failure limit [17]. The static loading model and uniform particle modeling designed by Rodriguez and Riera are the forerunners of the future reliability simulation of the particle contact method [18] [19]. From the several approaches above, the particle model for the flexural test pattern loaded at the two points above has not been widely discussed. The phenomenon of flexural stress is intriguing because it undergoes crack development that is challenging to anticipate in continuum modeling. Combining buckling and shear cracking causes particle contact to experience stress in the two main working planes. Therefore, the developed equation must be able to adopt the role of the particle bonding model, which can describe the behavior up to the collapse limit. On the other hand, the equation also adopts the response of the cement material, which is the essence of the bonding between particles, which can be substantially translated into the Mohr equation. Furthermore, this is why DEM is preferred to overcome the undiscovered condition in unreinforced beams, which is close to the phenomenon of brittle failure.

The purpose of this study was to model four-point concrete flexure testing using the DEM approach. The cohesive particle model was created using Yet Another Dynamic Engine

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(YADE) software and calibrated using experimental testing data, which was used as a building block to simulate the interaction between aggregate and cementitious materials. The DEM's ability to simulate flexural tests in 2D is shown. The resulting model can be used to predict the failure pattern of a flexural test structure and design the right mix proportion to match the desired flexural strength. So that material efficiency and concrete flexure testing time can be achieved.

2. Research Method

The research was started by preparing the tools and materials needed and then continued by testing the sieve gradation and the concrete's flexural strength. The results of the sieve gradation test were used to determine the particle diameter for DEM based on the results of the fineness modulus analysis. Meanwhile, for testing the flexural strength of concrete, it is used as a calibration for DEM testing. DEM modeling begins with forming a concrete geometry model and determining the particle material properties. Furthermore, external forces or loads must be applied to the concrete particles or elements to simulate the flexural test conditions. The application of Newton's law and the contact relationship between particles using the constitutive law model is applied to each particle. The position of the concrete element particles is updated based on the calculation of the interactions that occur between these particles. The modeling results will be calibrated and validated.

2.1 Experimental Test

Experimental testing was conducted at the Laboratory of Building Materials, Engineering Faculty, Yogyakarta State University. The tests carried out are sieve gradation and flexural tests.

2.1.1 Sieve Gradation

The sieve gradation test was carried out using ASTM C136 reference using a sieve shaker [20]. For coarse sieve grading, sieve numbers 37.5 mm (No.1 1/2) to 0.15 mm (No. 100) are used. Meanwhile, a 9.5 mm (No. 3/8) to 0.15 mm (No. 100) sieve is used for the fine gradation. The sieve gradation results in a soil size distribution curve [21].

Indian Standard determines the zone of fine aggregate concrete and calculates the fineness modulus (FM) by dividing the weight that passes through sieve no. 100, 50, 30, 16, 8, and 4 divided by the total weight of the fine aggregate [22].

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2.1.2 Flexural Test

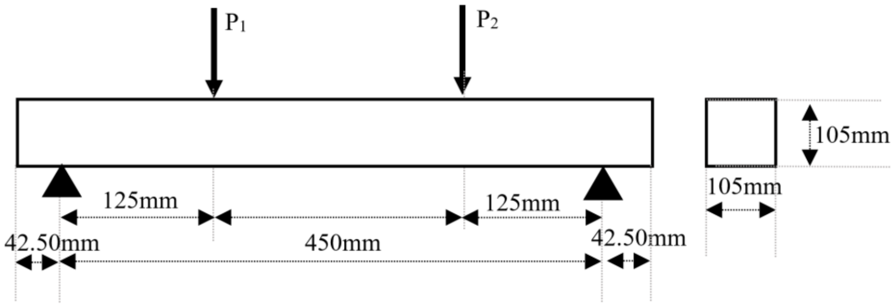
Before testing the flexural strength of concrete, it is necessary to state in advance the proportion of the concrete mix used. The concrete job mix is presented in **Table 1**.

Table 1. Mix Proportion.

Materials	Amount (kg/m^3)
Portland Pozzolan Cement	396
Fine aggregate	744
Coarse aggregate	1707
Water	181

Source: Author Research Design.

After determining the proportion of the concrete mixture, the flexural strength test of the concrete was carried out using ASTM D6272 with a four-point loading system [23]. The beam used has a length of 785 mm with a width and height of 105 mm, respectively. The location of the loading and concrete supports is presented in **Figure 1**.



Source: Author Flexural Test Design.

Figure 1. Setting-up of Flexural Testing.

2.2 Fundamental of DEM

2.2.1 Normal Strain

Normal strain in the Discrete Element Method (DEM) is the change in the relative distance between two or more particles in contact with the contact area [24]. To describe the kinematic contact of the particles, suppose there are two spherical particles, J and K, with centers PJ and PK (See **Figure 2**). When a particle link (cohesive or non-cohesive) is established between two particles, the link length (L) can be calculated using equation (1)

$$L = ||P_k^0 - P_k^0|| \tag{1}$$

Superscript 0 indicates the value at the period of linking the two particles. A normal strain (ε_N) is calculated based on the normal displacement (U_N) divided by the original length of the link (L), as shown in **Figure 2.**

$$\varepsilon_N = \frac{U_N}{L}$$

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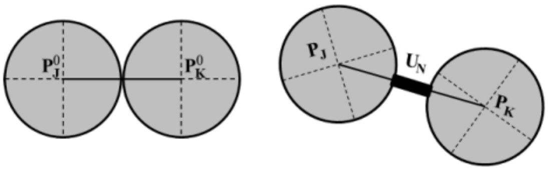


Source: Model Analysis for Particle (2023).

Figure 2. 2D Illustration of the Link.

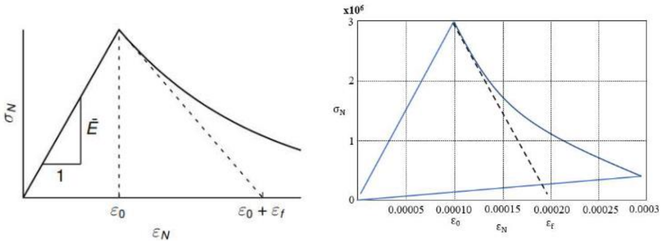
2.2.2 Stress on Normal Direction

The normal path constitutive law in a numerical simulation is influenced by 1D damage mechanics [24]. 1D damage mechanics is a method used to model material damage, assuming that damage occurs only in one direction or one dimension. The constitutive normal path law is used to describe the relationship between normal stress (σ_N) and normal strain (ε_N) using equation (2)

$$\sigma_N = [1 - \omega H(\varepsilon_N)]\bar{E}\,\varepsilon_N \tag{2}$$

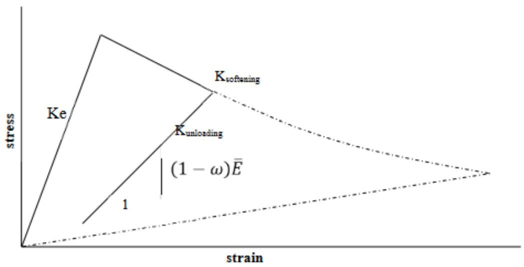
$$\omega = g(k) = 1 - \frac{\varepsilon}{k}\exp\left(-\frac{k-\varepsilon_0}{\varepsilon_f}\right) \tag{3}$$

Where E is the modulus (defines the elastic slope in the normal direction), the Heaviside function H (ε_N) deactivates the compression damage effect that corresponds physically to the crack closure. ω is the damage and effect of stiffness for unloading and reloading (tensile condition). ω is the variable defined on the damage evolution function's value (g), (k) is ultimate normal strain, (ε_0) is elastic limit strain, and (ε_f) is strain softening (See **Figure 3**). ω calculated by equation (3).



Source: modeling of the normal direction of the particle (2023).

Figure 3. Parameters of Materials in Normal Direction.



Source: modeling of the normal direction of the particle (2023).

Figure 4. Unloading and Reloading in Normal Direction.

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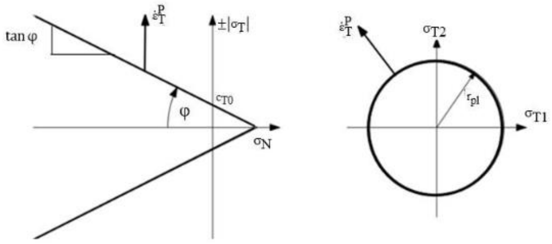
Where 0 describes the elastic limit strain (the product ε_0 equals the tensile strength of the links). ε_f is the initial softening slope in **Figure 4** and therefore controls the softening Branch of the particles.

2.2.3 Shear Stress

Constitutive law in the shear direction is declared by plasticity and defines shear stress (σ_T) in terms of shear strain (ε_T) [25].

$$\sigma_T = \bar{G}(\varepsilon_T - \varepsilon_T^P) \quad (4)$$

Where G is the shear modulus, which determines the elastic slope in the shear direction, ε_T^P The plastic shear strain.



Source: modeling for damage plasticity.

Figure 5. Plasticity Surface in Shear Direction.

Mohr-Coulomb plasticity expresses shear stress is limited as Equation (5).

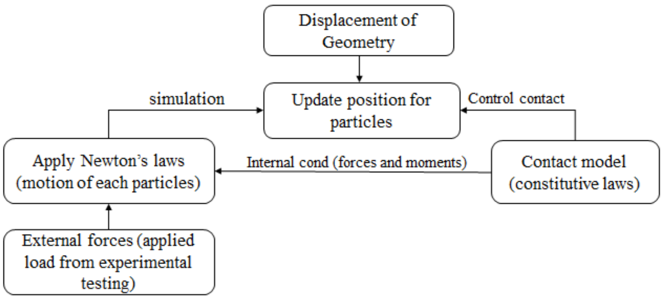
$$f(\sigma_n, \sigma_T) = \left| |\sigma_T| \right| - (c - \sigma_N \tan\varphi) \leq 0 \quad (5)$$

$$c = (1 - \omega)C_0 \quad (6)$$

C is cohesion, ω is the damage variable, and φ is the internal angle.

2.3 Modeling for Flexural Test

The simulations were carried out using the open-source code YADE [17]. YADE (Yet Another Dynamic Engine) is one of the software for DEM analysis written in C ++. Python is used in YADE as a user interface. In YADE, architecture is independent, including the form of particles or the input of new materials. In this study, the DEM analysis procedure is presented in **Figure 6.**



Source: Author Research Method (2023).

Figure 6. The procedure of DEM Analysis.

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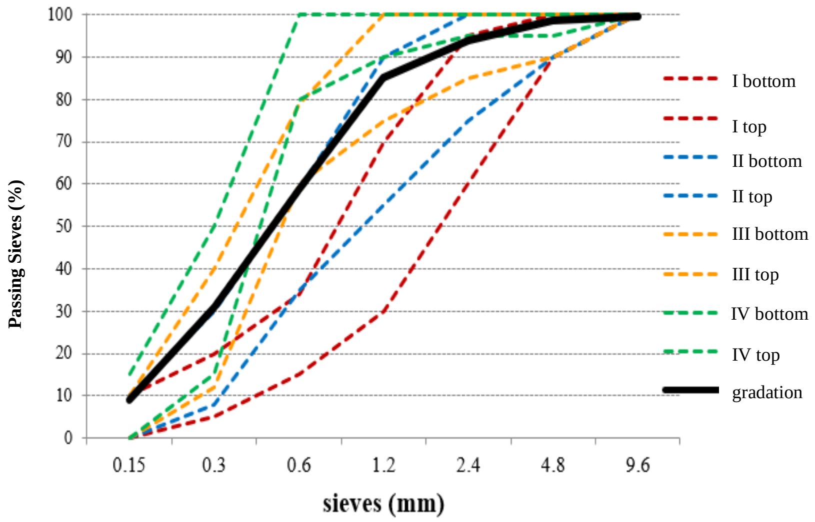
The DEM analysis procedure generally involves several steps, such as geometry displacement, where discrete particles are placed in a geometry or structure to be analyzed. After that, the interaction model between particles in the system is defined using constitutive laws that describe the mechanical properties of the particles, such as elasticity, strength, and resistance to damage. In addition, external forces or loads are exerted on the material under analysis. These forces or loads can come from experimental tests. The application of Newton's laws to each particle or element in the analysis is carried out. Newton's laws applied include Newton's law of motion and Newton's second law, namely the law of action-reaction. The positions of the particles or elements are updated based on the movements and interactions that occur between the particles or elements during the analysis.

3. Results and Discussions

3.1 Sieve Gradation

Based on the sieve gradation test for fine aggregate concrete, the size distribution of fine aggregate concrete is illustrated in **Figure 7.**



Source: Experimental Analysis (2023).

Figure 7. Fine Aggregate Gradation.

Based on **Figure 7**, it can be seen that the aggregate is included in the zone 3 gradation. In addition, a fineness modulus (FM) value of 2.239 is obtained, which meets the sand requirements of 1.5 - 3.8. The results of the coarse aggregate sieve gradation test are presented in **Figure 8**.

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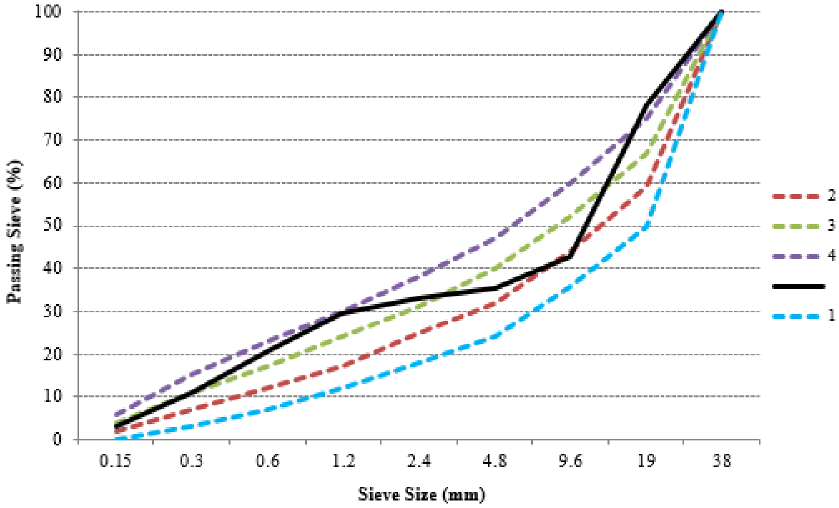

Source: Experimental Analysis (2023).

Figure 8. Coarse Aggregate Gradation.

The coarse sieve analysis test results with a sieve size of 0.15–50.8 mm obtained an FM of 7.27, which complies with SNI 7656:2012 for gravel of 5.0–8.0. Based on these results, the largest gravel size is 36.1 mm due to the cumulative percentage left behind from the previous sieve size of 17.584%, which is more than 5%, so the gravel size is taken from the top sieve, which is 36.1 mm.

The test results are then used to determine particle dimensions in the DEM model. The prediction was used based on several trials of particle dimensions in the simulation, which were divided into two categories, the average coarse and fine aggregate (starting from ten millimeters to thirty millimeters in diameter) with spherical material. The diameter in the analysis was determined to be ten millimeters with a total of ten thousand uniform spherical particles.

3.2 Flexural Test

The beam used is normal concrete with a quality of 25.13 MPa which was subjected to a flexural test with the results presented in **Table 2**.

Table 2. Flexural Test Results.

Code	Height (mm)	Width (mm)	Length (l) (mm)	Distance Between Supporting System	Weight (Kg)	Load (N)	Experimental Flexural Strength (N/mm²)	Numerical Flexural Strength (N/mm²) DEM
L_1	105	105	504	450	12,9	14660	5.70	5,68
L2	105	100	505	450	12,5	14800	7.12	6,11
			Averages				6.75	5,89

Source: Author Analysis (2023).

The flexural strength test results in **Table 2** are used to calibrate DEM testing. On a laboratory scale, it is important to know the readings of load and deflection diagrams in brittle

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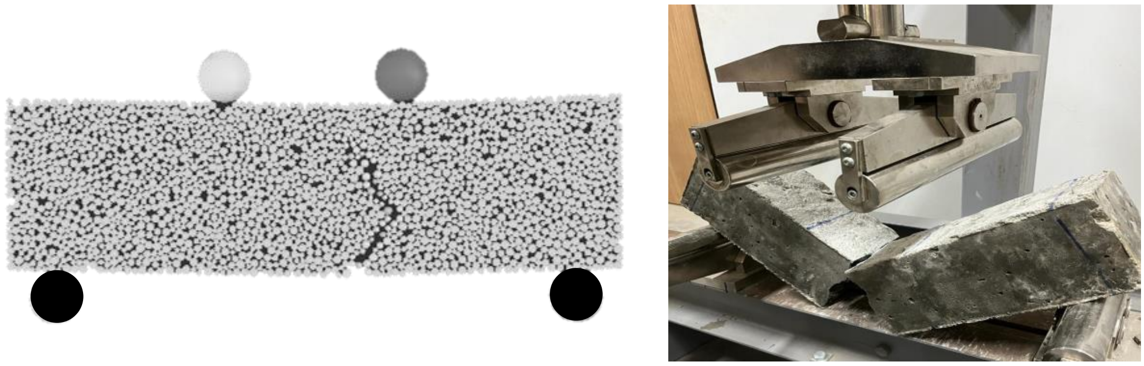
materials (without reinforcement). The resulting values are converted into stresses and strains between particles which affect the bending damage pattern of the beam as a result of numerical analysis.

When compared with the numerical flexural test (DEM) results, the difference in the test results is 2.13%, which means that the modeling results meet the test requirements. In this test, the amount of displacement cannot be measured due to brittle failure, and the linear variable differential transducer cannot be applied due to safety factors.

3.3 Numerical Modelling

The concrete material used has E = 30GPa, material density ρ = 2500kg/m^3; the average concrete compressive strength is 25.13 MPa, and the average splitting tensile test is σt = 2.86 MPa. The amount of load capacity that can be borne by 8763.4 N. The failure phase begins with the elastic part, then cracks and collapses. The parameters used for the boundary conditions are v = 0.2, γ = 1.4, Φi = 20^o, and β = 120.



(a) (b)

Source: Author Analysis Results (2023).

Figure 9. (a) Numerical Flexural Test; (b) Experimental Flexural Test.

The phenomenon of inter-particle cracking is caused by excessive stress (S3), which causes the particle contact to weaken and break. A 2 Dimension discrete element model is simulated to reveal the impact of particle contact on quasi-static dynamic loading up to the collapse limit. At a shear strain of 0.9, it can be seen that there is a change in particle behavior starting at a stress of 3.5 MPa, causing a shift in the spherical particles studied.

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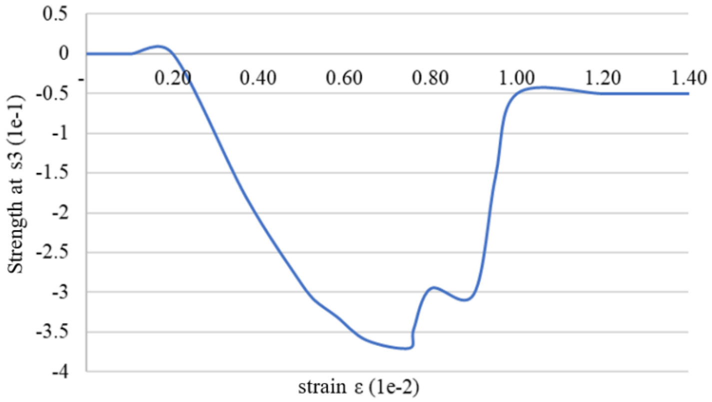

Source: Author Analysis Results (2023).

Figure 10. Crack Coalescence on Round Particles.

The contact begins to weaken, and cracks open in the same area under elastic loading, although the ITZ phenomenon is not specifically disclosed [17] [26]. At this stage, the ultimate particle contact strength is based on the magnitude of the resistance or shear strain value because high local softening must be used to compensate for the free rotation.

4. Conclusion

The discrete element method (DEM) approach has described a new phenomenon in simulating crack behavior in flexural testing of unreinforced concrete. The DEM results revealed only a 2.13% difference in the experimental results of the flexural strength test. Meanwhile, crack behavior can be observed directly in the DEM simulation. The results of this study can be used to predict the failure pattern of a flexural testing structure before carrying out experimental tests, as well as to design the right proportions so that flexural strength can be achieved. So that material efficiency and concrete flexure testing time can be carried out.

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