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Validation of Experimental Results using Software Based on DEM

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Abstract— *Present study deals with the modelling of the compressive strength with different porosity for hardened concrete by using Discrete Element Method. A brief description of the Discrete Element Method and the process of the model development for uniaxial compression test of a hardened concrete cube is mentioned in the given paper. The aim of the study is to simulate the material behavior and validate the parameters by comparing it with experimental data using the trail version of Particle Flow Code* (PFC_{3D}) *which is a commercial software based on DEM.*

Keywords: Discrete Element Method, concrete, stress-strain, compressive strength, Particle Flow Code

Introduction

Discrete Element Method (DEM) is a group of numerical methods for computing the mechanical behavior of materials or structures consisting of a large number of particles. Structural components comprise of granulated material or bricks, and which are not connected to each other at particle level. DEM is, therefore, mostly used to model grains, soil, fractured rock, masonry structures like domes and arches. DEM is used extensively to study granular media of no cohesion [1], rock [2], geotechnical and geological studies [3],[4], for the interaction of granular media (soil and rock) [5]. In the last two decades the DEM has been successfully applied in various areas of mining, powder metallurgy, civil engineering and in the oil industry. Recently, DEM is also used for the modelling of the behaviour of fresh concrete [9], [10] and hardened concrete [11].

A numerical technique is said to be a discrete element model if:

- It consists of separate, finite-sized bodies (discrete elements) and each of those elements are allowed to displace independently.
- The displacements of the individual elements can be large.
- The elements are free to be in contact or loose contact with each other [6].

With advances in computing power, it has become possible to numerically simulate millions of particles on a single processor [7].

In DEM, the discrete assemblage of particles make it attractive for modeling large deformation problems in fresh concrete engineering. Although computer simulated experimentation using the DEM was originally developed, as a tool, for examining geotechnical problem, but it can be used in multiple areas of structural engineering and research problems. Before any modeling is attempted suitable model parameters should be chosen for a realistic model.

The distinct element method is a version of DEM proposed by Peter A. Cundall in 1971 [8]. In this method every particle is considered as a perfectly rigid element and the behavior of this element is expressed by the equations of motion of extended bodies. A spring is provided between rigid elements which make contact with each other so as to express the interaction of force between them. Then, the equations of motion of each rigid element are solved by numerical integration along the time axis, whereby the behavior of the element is analyzed. The time integration method works with the central difference method, an explicit solver.

Modelling with DEM

For the present study, trial version of commercially available DEM software package, the Particle Flow Code (PFC3D) of Itasca was used, which is based on the following theoretical assumptions:

- The particles are treated as rigid bodies.
- The fundamental particle shape is a {disk with unit thickness in 2D; sphere in 3D}, denoted ball.
- The clump logic supports the creation of rigidly attached {disks with unit thickness in 2D; spheres in 3D}, denoted pebbles. Each clump consists of a set of overlapping pebbles that acts as a rigid body with a deformable boundary. Clumps may be of arbitrary shape.
- Particles interact at pair-wise contacts by means of an internal force and moment. Contact mechanics is embodied in particle-interaction laws that update the internal forces and moments.
- Behavior at physical contacts uses a soft-contact approach where the rigid particles are allowed to overlap one another at contact points. The contacts occur over a vanishingly small area (i.e., at a point), and the magnitude of the overlap and/or the relative displacement at the contact point are related to the contact force via the force-displacement law.
- Bonds can exist at contacts between particles.
- Long range interactions can also be derived from energy potential functions.

The assumption of particle rigidity is a good one when most of the deformation in a physical system is accounted for by movements along interfaces. The deformation of a packed-particle assembly (or a granular assembly such as sand), as a whole, is well-described by this assumption, since the deformation results primarily from the sliding and rotation of the particles as rigid bodies and the opening and interlocking at interfaces, not from individual particle deformation. Precise modeling of particle deformation is not necessary to obtain a good approximation of the mechanical behavior for such systems.

In addition to traditional particle-flow applications, PFC can also be applied to the analysis of solids subjected to prescribed boundary and initial conditions. In such models, the continuum behavior is approximated by treating the solid as a compacted assembly of many small particles. Measures of stress and strain rate can be defined as average quantities over a representative measurement volume for such systems. This allows one to estimate interior stresses for granular materials such as soils, or solid materials such as rock or plastics formed by powder compaction.

In addition to balls and clumps, the PFC particle-flow model also includes walls. Walls allow one to apply velocity boundary conditions to assemblies of balls or clumps for purposes of compaction and confinement. The balls, clumps, and walls interact with one another via the forces that arise at contacts. The equations of motion are satisfied for each ball and clump. However, the equations of motion are not satisfied for each wall (i.e., forces acting on a wall do not influence its motion). Instead, its motion is specified by the user and remains constant regardless of the contact forces acting on it. Also, contacts may not form between two walls; thus, contacts are ball-ball, ball-pebble, pebble-pebble, ball-facet, or pebble-facet. Figure 1 shows the DEM cycle taking place in PFC3D.

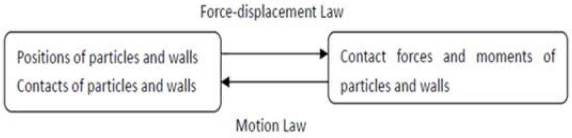


Figure 1. Procedure of each DEM calculation cycle

Material Genesis

In the present study the compression stress-strain performance of a concrete was modelled with PFC and was verified with work done by Deo & Neithalath (2011) [12]. They performed group of experiments on various types of aggregate and void ratios. Based on their experimental results PFC models are prepared using parallel bond and validated here with desired porosities.

The concrete was modelled with a large number of discrete elements, each of them being spherical. The element diameters in the model of the concrete cube were based on the aggregate sizes used in the real material. In the model the actual particle size distribution of the aggregate used for the reference concrete was intended to approximate. The particle size distribution was compiled from the applicable grading limit curves for 25.4 mm maximum particle size aggregate, taking into account the minimum demand of cement paste (void volume) of the fully compacted aggregate bulk.

The particle size distribution of the original material is given in Table 1

Table 1. Particle size proportions

Mix	Aggregate Size		Fine Aggregate	Void Ratio (Ø)	
	Passing (mm)	Retained (mm)		Designed	Obtained
M-1-1 (1/2”)	25	12.5	Nil	0.19	0.164
M-1-2 (1/2”)	25	12.5	Nil	0.22	0.245
M-1-3 (1/2”)	25	12.5	Nil	0.27	0.261

M-2-1 (3/8”)	12.5	9.5	Nil	0.19	0.195
M-2-2 (3/8”)	12.5	9.5	Nil	0.22	0.238
M-2-3 (3/8”)	12.5	9.5	Nil	0.27	0.246

The particle sizes were created and the volume of fractions was set regarding the particle size distribution of the original aggregate material. During this phase of the modelling one has to specify five parameters to every fraction:

1. The minimum radius of the material in the fraction.
2. The radius ratio; that is the ratio of the maximum to the minimum radius.
3. The ratio of the volume of the particles in the given fraction, related to the total volume.
4. The distribution type of the given fraction. In the present study the fractions are uniformly distributed.

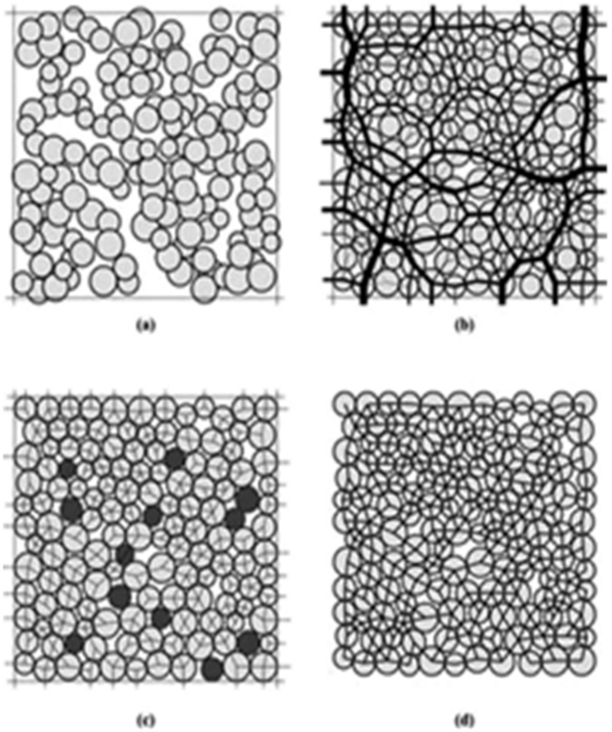


Figure 2. Material genesis procedure: (a) particle assembly after initial generation but before rearrangement; (b) contact force distribution after the second step; (c) Floating particles and contacts after the second step; (d) parallel-bond network (PFC3D User’s Guide, 2008)

The algorithms are built in the software into a given storage of supporting algorithms, called Fishtank, which uses FISH programming language used in PFC3D. To model concrete Material-Genesis Procedure was used, which generates a material consisting of grains and cement (PFC3D User’s Guide, 2008). During this procedure (Figure 2) initially an assembly is created, in which the particles are arranged randomly (having a desired porosity) with a much smaller radius than the required and without particle overlapping. Then, the particle radii are gradually increased to their final values and the system is allowed to reach static equilibrium under zero friction. Then the radii of the particles are changed uniformly to achieve a specified isotropic stress (mean value of the three principal stresses). This is a typically low value relative to the material strength (less than 0.01% of the uniaxial compressive strength). After the first two steps an assembly of randomly placed particles with non-uniform radii is produced. These assemblies can contain a large number of floating particles (those which have fewer than three contacts). It is desirable to reduce number of such elements, in order to obtain a denser network of bonds. After all of the contact bonds and parallel bonds are installed, the specified friction coefficient is assigned to the contacts. The material vessel can be removed and the specimen can be used for a boundary-value simulation or it can be subjected to material testing. This widely applied procedure was followed in the investigations introduced in the present paper.

Parameter Settings

The in-built functions generated initially can help to create initial geometry faster, but to achieve a satisfactory result, it is required to set the precise contact material parameters. The most influential parameters that affect the behavior of the model are the density of the balls, the friction coefficient in the unbonded contacts, as well as the shear and normal stiffness and strength of the bonds. To set up the parameters appropriately, a uniaxial compression test in PFC3D was performed and compared with the experimental results.

a) Density: As per the data reported by the Deo & Neithalath (2011) [12] actual values of the density incorporated in the PFC model.

b) Void ratio: As per PFC manual the void ratio are calculated as per the grain distribution, it is not taking in account the amount of matter filled by the cement paste. To incorporate the cement paste a modified void ratio value is assigned to the assembly based on the following expression:

Basic expression of Void ratio

$$\emptyset = \frac{Vv}{V} \tag{1}$$

$$Vv = V - (Va + Vp) \tag{2}$$

In PFC,

$$Vv\,(PFC) = V - Va \qquad (3)$$

(As per expression (3) volume of paste is not included in the calculation of void ratio in PFC.)

We have

$$Vp = Vc + Vw \qquad (4)$$

(Volume of water can be neglected as it is very small)

$$Vp = Vc \qquad (5)$$

Aggregate cement ratio,

$$\frac{A}{C} = \frac{Va}{Vc}$$

$$Vv = V - (Va + Vc) \qquad (6)$$

From expression (1)

$$\emptyset = \frac{V-(Va+Vc)}{V}$$

$$\emptyset = 1 - \frac{Va(1+\frac{C}{A})}{V} \qquad (7)$$

Expression (7) gives a relationship between PFC porosity with actual porosity based on aggregate-cement ratio.

$$\emptyset\,(PFC) = 1 - [\frac{(1-\emptyset(actual))}{(1+\frac{C}{A})}]$$

Where,

- Void ratio

Vv - Volume of void

Vc – Volume of cement

Vw – Volume of water

A/C – Aggregate-Cement ratio

V- Total volume of sample/ container.

c) Other parameters:

Following parameters are set according to the property of the material taken under consideration.

- Bulk modulus = 4.50x10^9 N/m²
- Friction coefficient =0.4

Parameters of the parallel bonds:

- The mean value of the normal strength = 3.0x 10^7 N/m²
- The standard deviation of the normal strength = 9.0x 10^6 N/m²
- The mean value of the shear strength = 9.0 x 10^6 N/m²
- The standard deviation of the shear strength = 27.0x 10^5 N/m²
- The stiffness ratio of the parallel bonds = 2.5

Compression Test

The compression test can be simulated by the built-in functions of the PFC software pre-programmed in the Fish-tank, and the user can calibrate the test to the actual specimens of interest. The process is as follows. First the sidewalls of the sample are deactivated. The sidewalls of the sample can be selected and assigned to the software and the test can be done along all three axes. The friction of the remaining walls is set to value higher than that of sidewalls, because in case of the real test on the compression testing machine in the lab conditions, the friction between the loading plate and the sample is high. The bottom wall is fixed and the top wall presses the sample with a given force or velocity until it destroys the sample. The results of the compression test were used to calibrate the models. Figure.3 shows the compression test in PFC$_{3D}$.

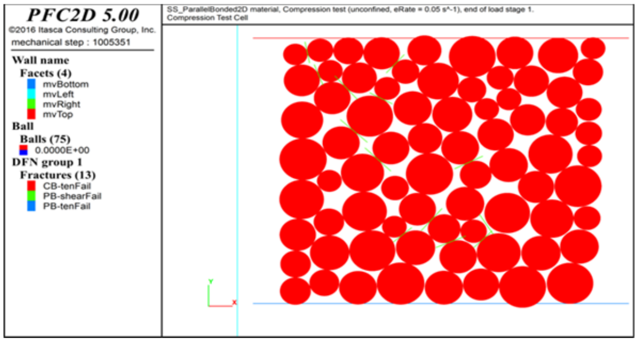


Figure 3. Compression test of PFC model

Results.

The final values of the parameters of the DEM model were reached after several iteration steps.

NOTE-The PFC (trial version) software generates the result in the form of image and does not give the values for the same. The graphs shown below are the images of the output generated.

(a) Aggregate size -1/2” (Passing 25mm sieve, retained on 12.5mm sieve)

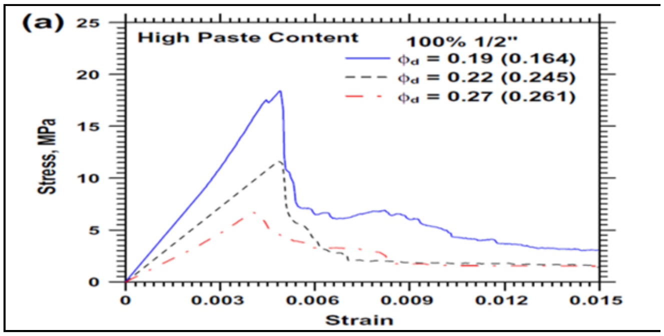
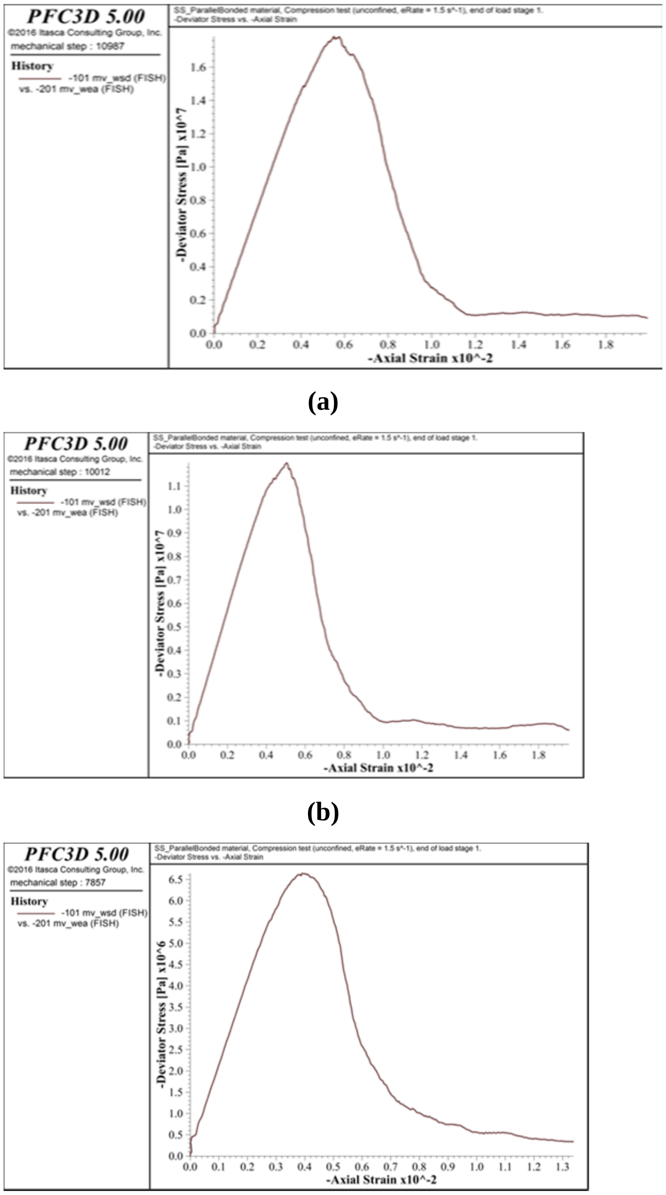


Figure 4. Stress-Strain plot for ½" Aggregate (Deo & Neithalath-2011)



(a)

(b)

(c)

Figure 5. Stress-Strain PFC plot ½" Aggregate

(a) $Ø_d$ =0.19, (b) $Ø_d$=0.22, (c) $Ø_d$=0.27

b) Aggregate size -3/8" (Passing 12.5mm seive and retained on 9.5mm sieve)

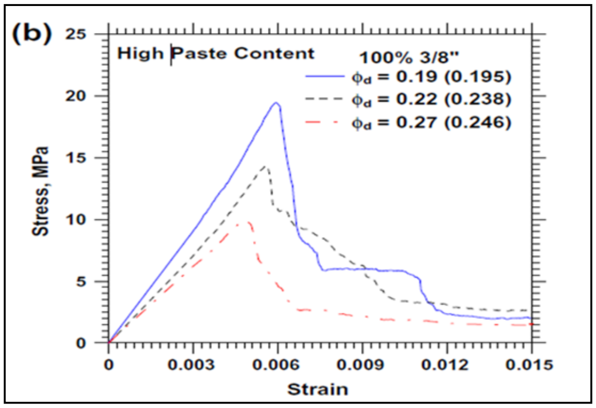
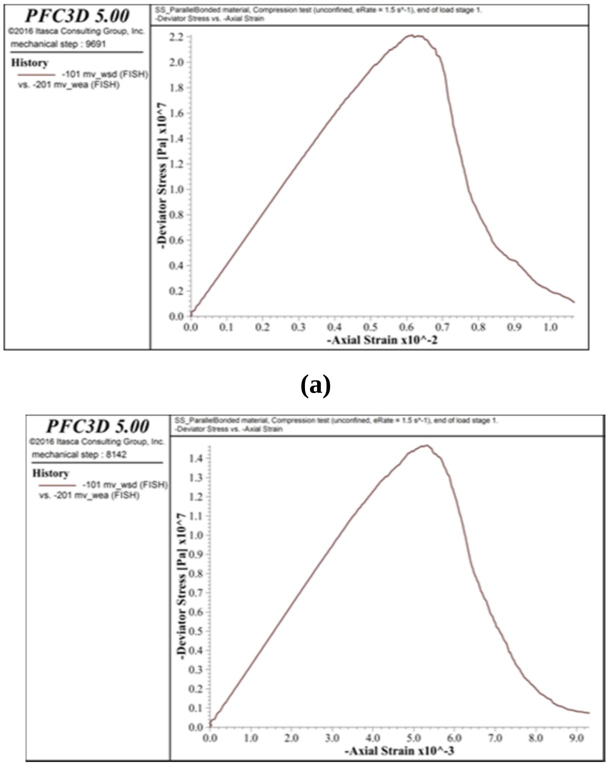
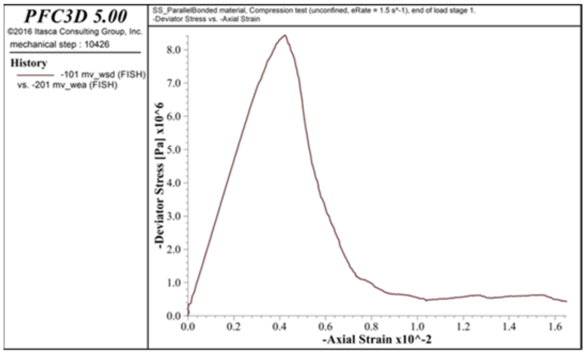


Figure 6. Stress-Strain plot for 3/8" Aggregate (Deo & Neithalath-2011)



(a)

(b)



(c)

Figure 7.Stress-Strain PFC plot for 3/8” Aggregate

(a) Ød =0.19, (b) Ød=0.22, (c) Ød=0.27

It can be concluded from Figure 5 and 7 that the peak values of stress-strain given by PFC model matches with experimental results for different values of void ratio. PFC (corrected) porosity values are matching with the experimental values. Also as the size of aggregate increases the peak value of stress increases, both in PFC as well as experimental results.

6. Conclusion

It is shown– based on the evaluation of a numerical simulation and experimental verification – that Discrete Element Method (DEM) is capable of modelling the uniaxial compression testing method of hardened concrete cube specimens, and after a sufficient parameter set up, the model can lead to results that are correlated to real laboratory test observations. Compressive strength, Young’s modulus and stress-strain response can be reproduced. With the help of DEM modelling, the laboratory test procedures can be easily simulated and the numerical tests can be repeated multiple times to follow random material behaviour. Statistically reasonable results can be created without the need of a large companion of laboratory tests that may add to the better understanding of material behaviour and failure process of hardened concrete.

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