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Application of the discrete element method for the simulation of size effects in concrete samples

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ABSTRACT

This study aims to determine the validity of the discrete element method in predicting the size effect of cylindrical concrete samples under compression. For this purpose, a series of simulations are carried out on a set of particle assemblies with different diameters and aspect ratios. A fixed particle-size distribution and a single set of model parameters are used for all numerical simulations. Using compressive peak stress, peak strain and stress–strain curve as reference, numerical results are compared with experimental observations. The discrete element model is shown to effectively reproduce the effect of aspect ratio on compressive properties. On the other hand, although the method succeeds to capture the so called 'wall effect', it fails to show good correspondence with experimental values due to the assumption of spherical particles. The effect of end friction is also addressed. These findings give insight into the scalability of discrete element models when used for the simulation of concrete material.

1. Introduction

When it comes to the size effect of concrete, many studies have shown that the mechanical properties found through experimentation, depend on the geometry and the boundary conditions of the sample being tested. While the effect of boundary conditions takes the form of end friction, the effect of geometry presents itself as the height-to-diameter ratio (aspect ratio) and the diameter-to-aggregate size ratio of the sample (Sim et al., 2013).

The work of Van Mier et al. (1997) is a comprehensive study on size effect, where the influence of aspect ratio (slenderness) and boundary condition on strength and the overall stress–strain curve is examined. The general conclusion draw from this study is that a lower slenderness and a higher end-friction lead to higher strength and a more ductile post-peak response. In another comprehensive study, this time by Sim et al. (2013), the compressive strength of concrete samples with varying diameters, aspect ratios and maximum aggregate sizes were compared. Their results show that by independently increasing the diameter and aspect ratio of the test sample, the value of strength will decrease. Conversely, if diameter and aspect ratio are kept constant, by increasing the maximum aggregate size, the value of strength will increase. Sinaie et al. (2015) carried out a series of experiments to determine the effect of size on the response of concrete samples under monotonic and cyclic loading. Their results show the dependency of compressive strength f_c, peak strain ϵ_c and initial modulus E_c on the diameter and aspect ratio of the sample being tested. In addition, their results also demonstrate that as the diameter and aspect ratio of the sample decrease, test results exhibit higher scatter. Roddenberry et al. (2011) investigated the effect of end friction on the failure of cylindrical concrete samples. Their results show that having higher friction not only leads to higher strength values but also affects the crack pattern. Moreover, by carrying out compression tests using a force-control setup and taking advantage of a high-speed video camera, they conclude that higher end-friction results in more sudden failure.

When it comes to the simulation of granular material such as concrete, the discrete element method is a reliable approach due to its particle-based nature. On the other hand, the computationally expensive nature of this approach is being overcome with the increasing processing power of computers along with parallel programming paradigms (Zheng et al., 2012). Hentz et al. (2004) investigated the effectiveness of discrete element models in predicting the dynamic response of concrete samples. Azevedo et al. (2008) used the discrete element method for the simulation of concrete. They used a multi-phase model by making a distinction between the particles that represent aggregates and those that represent the cement matrix. The analyses were carried out on 2D models in tension and compression, whereby it was concluded that a more accurate simulation

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of concrete behavior can be obtained by using a ductile failure model in tension and by incorporating friction into the simulation. Shiu et al. (2008) applied the discrete element method to simulate the penetration of missiles into concrete slabs. Kim and Buttlar (2009) investigated the effectiveness of discrete element models to predict fracture in asphalt concrete. Tran et al. (2011) applied the discrete element method to simulate concrete under triaxial loading. Once calibrated through uniaxial and triaxial experimental results, they demonstrated that the local interactions within the model can properly explain the macroscopic behavior of a sample under confining pressure. Using the discrete element method, Huang et al. (2014) and Kuhn and Bagi (2009) investigated the effect of size on soil samples. Rojek et al. (2012) studied the utilization of localized interaction parameters as opposed to a global set of parameters for the entire assembly. They concluded that as the heterogeneity of the material increases, a global set of parameters cannot be used for all of the particles, and the interaction parameters between two particles should be set according to the geometry of the two particles being paired. Oñate et al. (2015) developed a detailed local constitutive model for particle interactions. Using experimental results for validation, they illustrated the effectiveness of the approach for the simulation of cement and concrete. Sinaie et al. (2016) used 2D discrete element models to study the effect of thermal incompatibility on the degradation of concrete samples. Combined implementation of the discrete element and finite element methods have also been utilized for material simulation (Xu and Zang, 2014; Haddad et al., 2016).

The geometry and boundary conditions of a concrete sample can be viewed as properties of that sample's structural form. As mentioned in the beginning, the compressive strength measured in the laboratory depends on the geometry and the boundary conditions of the sample being tested. This indicates that the strength value being determined by compressive testing is as much a structural property as it is a material property. Ideally, if a pure material model were to be established for concrete, it should be independent of the geometry and boundary conditions of the sample itself. This paper aims to determine whether the discrete element method satisfies this requirement, and to what extent. In other words, the aim is to determine whether a single set of material properties is sufficient for a discrete element model to numerically capture what is known as the 'size effect'.

2. Multi-phase discrete element model

This section describes the formulation of the discrete element model used in this study. In what follows, the interaction between any two particles is either categorized as a *contact* interaction or as a *cohesive bond* interaction. Contact interactions can dynamically form or break during an analysis, but cohesive bond interactions are created at the beginning of the simulation and if broken during the analysis, the interaction is permanently lost. Moreover, contact interactions form when two particles touch each other, while cohesive bond interactions are created when two particles are in close proximity to one another at the beginning of the analysis (but might not necessarily be touching).

In addition, this study makes a distinction between particles representing aggregates and those representing the mortar matrix. This is in contrast to single-phase models (Tran et al., 2011; Oñate et al., 2015) where all particles are taken to be of the same material. The main difference between the two types of particles lies in the fact that in an entire assembly, only mortar particles can have a cohesive bond with their adjacent particles. In the following text, where parametric values are mentioned, properties associated to aggregate particles and mortar particles are distinguished by using the subscripts 'a' and 'm'.

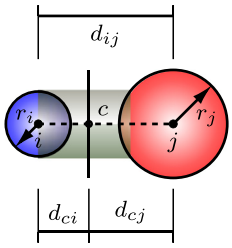

Fig. 1. Cohesive bond between a mortar matrix particle (blue) and an aggregate particle (red). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.1. Kinematics of cohesive bond interactions

As mentioned before, cohesive bonds are created only at the start of the simulation. Moreover, for a cohesive bond to be assumed between two particles, the two particles have to be in close proximity of each other, and at least one of them has to be of mortar type. Cohesive bonds are assumed to be in a state of zero stress when they are created. However, during the analysis, they can carry normal forces (in compression and tension) as well as shear and moment. Note that existing bonds can break (permanently) during the simulation, however, new cohesive bonds are never created once the simulation has started.

The condition for a bond between two particles i and j is:

$$\frac{|\mathbf{d}_{ij}|}{r_i + r_j} \leq 1 + \gamma \tag{1}$$

where $\gamma > 0.0$ is a parameter that allows a bond to be established between two particles that are in close proximity but are not in perfect contact. Moreover, in Eq. (1), $\mathbf{d}_{ij} = \mathbf{x}_j - \mathbf{x}_i$ is the distance between the centroids of particles i and j, as illustrated in Fig. 1.

The distance between the centroid of particle i and the contact point c is denoted by the vector $\mathbf{d}_{ci}$ and is equal to:

$$\mathbf{d}_{ci} = \mathbf{d}_{ij}\left(\frac{r_i}{r_i + r_j}\right) \tag{2}$$

The cross section of the bond area is assumed to be:

$$A_{ij} = \pi[\min(r_i, r_j)]^2 \tag{3}$$

The approach taken here to determine the deformations experienced by the bond throughout a simulation, relies on the initial orientation of the particles when the bond is created. Therefore, for every cohesive bond interaction that is created, the initial position ($\mathbf{x}_0$) and orientation ($\boldsymbol{\theta}_0$) of the two particles are saved into memory and utilized over the analysis. Using these stored values, the displacement and rotation of each particle up to time t, relative to its initial state, become $\Delta\mathbf{x} = \mathbf{x}_t - \mathbf{x}_0$ and $\Delta\boldsymbol{\theta} = \boldsymbol{\theta}_t - \boldsymbol{\theta}_0$.

Therefore, the displacement of the contact point on particle i is:

$$\Delta\mathbf{x}_{ci} = \Delta\mathbf{x}_i + (\mathbf{d}_{ci} \times \Delta\boldsymbol{\theta}_i) \tag{4}$$

and the relative displacement between the contact points on the two particles becomes $\Delta\mathbf{x}_{c,rel} = \Delta\mathbf{x}_{cj} - \Delta\mathbf{x}_{ci}$.

The unit normal vector of a cohesive bond is defined as:

$$\hat{\mathbf{n}}_{ij} = \mathbf{d}_{ij}/|\mathbf{d}_{ij}| \tag{5}$$

and consequently, the unit shear vector is:

$$\hat{\mathbf{s}}_{ij} = \frac{\Delta\mathbf{x}_{c,rel} - (\Delta\mathbf{x}_{c,rel} \cdot \hat{\mathbf{n}}_{ij})\hat{\mathbf{n}}_{ij}}{|\Delta\mathbf{x}_{c,rel} - (\Delta\mathbf{x}_{c,rel} \cdot \hat{\mathbf{n}}_{ij})\hat{\mathbf{n}}_{ij}|} \tag{6}$$

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