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A discrete element model of concrete for cyclic loading

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ABSTRACT

This paper takes advantage of the discrete element method to develop a model of concrete for cyclic simulations. For this purpose, a micro-mechanical damage model that also allows stress-reversals is formulated for inter-particle bonds. Moreover, a multi-phase implementation of the discrete element method is developed and used for two distinct reasons. First, to characterize aggregate and mortar particles separately. Second, to allow the effect of the interfacial transition zone to be taken into account. A strict validation approach is taken in this work, whereby the developed model is only calibrated against monotonic stress-strain curves and then evaluated for its performance under cyclic loading. Simulation results are constantly compared against experimental values. These comparisons illustrate the capability of the model to predict cyclic properties of concrete. Progression of damage is discussed in terms of numerical variables and also through the visualization of force chains and crack propagation.

1. Introduction

With the widespread use of concrete as a construction material in earthquake-prone regions, characterization of the cyclic properties of concrete has been the subject of many studies. These involve a range of experimental investigations carried out on plain concrete under cyclic loading [1–7]. As two of the pioneering contributors, Bahn and Hsu [1] characterized some important features of concrete under cyclic loading. What sets aside Bahn and Hsu's [1] work is the fact that they also examined these features in relation to random cycles and evaluated the existing analytical models against such loadings. To make cyclic models of concrete applicable to the design of spirally reinforced concrete columns, Sakai and Kawashima [2] investigated the behavior of confined concrete under cyclic loading.

As computational methods for simulating concrete structures were evolving, Sima et al. [3] aimed to improve the constitutive model of concrete that was being used in such computational methods, especially in relation to the smeared crack approach. Their constitutive model covered the cyclic behavior of concrete in the compressive and tensile regions and employed separate damage parameters for each region. The constitutive model of Sima et al. [3] has been improved by Breccolotti et al. [6] for a more accurate account of damage accumulation.

More recently, Sinaie et al. [7,8] investigated the cyclic response of cylindrical concrete samples in the context of size effects and in combination with temperature effects. Aside from its standard use, concrete is also a main load-bearing component of many composite systems. Studies involving fiber-reinforced concrete [9] and concrete-filled tubes [10] have also dealt with the characterization of concrete under cyclic loading.

When it comes to the simulation of concrete, meshless methods have shown to have certain advantages. This is especially true in relation to discontinuities (cracks), where such methods allow simple yet reliable formulations for the initiation and propagation of cracks. For example, Rabczuk and Belytschko [11] and Rabczuk et al. [12] incorporated their idea of representing cracks as a set of contiguous particles to simulate a range of 3D concrete problems involving static and dynamic loading with rate-dependent and independent material models. In their model, the crack surface is not restrained by the topology of the model, since the formation of a crack and its direction is determined by the failure criterion at the particle scale. Rabczuk et al. [13] later extended modified this approach by splitting the particles where cracking is detected. Doing so eliminated the need for additional variables at the location of the crack, therefore simplifying the formulation.

Being a mesh-free particle-based method, the discrete element method (DEM) has also shown to be a reliable approach for the simulation of concrete. The DEM has also been coupled with other computational methods such as smooth-particle hydrodynamics (SPH) [14] for problems involving fluid-structure interaction and

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computational fluid dynamics (CFD) for problems involving flow in porous material [15].

As one of the most earliest works, Cundall and Strack [16] evaluated a 2D DE model of packed disks. Although primarily aimed at granular assemblies such as sand, their work set the stage for the development of a computation model allowing interactions to be set at a particle scale, and therefore, applicable to various granular material. Due to its generality, aside from being extended into 3D and the addition of inter-particle bonds, the underlying concept of the discrete element method has not changed over the years. The main advancements made to the discrete element method have been in the direction of its applications, and the computational implementation, which in turn allows larger scale (or higher resolution) applications. At the time, Cundall and Strack [16] highlighted that their approach would allow a 1500-particle assembly to be simulated using no more that 64 kB of memory. Nowadays, simulations involving tens of thousands of particles is the norm and can easily be carried out on regular desktop computers.

With the inclusion of inter-particle bonds into the DEM, such models have shown to be an effective solution to problems involving fracture [17–20]. This includes the simulation of concrete, as fracture and crack propagation play an important role in the behavior of this material. Hentz et al. [21,22] defined an interaction range as a criterion to establish inter-particle bonds (referred to interaction links in their work) between neighboring particles. With this method, they created particle assemblies to investigated the effectiveness of DE models in predicting the static [21] and dynamic [22] properties of concrete samples. Using a similar approach, Shiu et al. [23] used the discrete element method to simulate the penetration of missiles into reinforced concrete slabs. Aside from the particles that represented the concrete, they also included the reinforcement bars as a series of aligned particles and the impacting missile as a rigid assembly of particles. Note that the properties of these different materials are implemented into the model through the mechanical properties of the inter-particle bonds, which they referred to as parallel bonds.

Up to this day, most researchers take a single-phase approach to their DE simulations, meaning that they have one single type of particles and one single type of bond between the particles. In contrast to this, Azevedo et al. [24] implemented a multi-phase approach to make a distinction between the aggregates and the cement matrix. Doing so gives the possibility to have a different sets of mechanical parameters (or even constitutive relations) depending on the type of the particles that exists at the two ends of the bond. Specifically for concrete, this means that the model can take into account three different phases corresponding to aggregate-aggregate, aggregate-mortar, and mortar-mortar bonds. Using this multi-phase approach, Sinaie et al. [25] investigated the thermal degradation of concrete from the standpoint of incompatibility between aggregates and the mortar matrix in terms of their coefficients of thermal expansion.

Studies involving DE models of concrete have mostly dealt with monotonic loading, whereby micro-mechanical properties (defined at particle-scale) have been shown to properly translate into macro-mechanical characteristics (observed at sample-scale). However, this translation is yet to be shown for loading histories that involve stress reversals. To fill this gap, the present study explores the advantages/disadvantages of the DEM when it comes to simulating concrete under cyclic loading. To this end, a damage-based inter-particle bond model is developed to accommodate stress reversals and to take into account the degradation of micro-mechanical properties in compression, tension and shear. A multi-phase approach is also taken here, whereby the interfacial transition zone (ITZ) and the material weaknesses associated with it are introduced into the model. The numerical samples created and analyzed here are based on a series of laboratory experiments carried out by the author in a previous study [7]. To avoid the imposition of an strenuous calibration requirement, material properties of the multi-phase DE model are calibrated against a fraction of the experimental results, and the remaining experimental data are used to validate the calibrated model. These validations clearly demonstrate the capability and reliability of the DEM for the simulation of concrete specimens under cyclic loading.

It is important to note that the present paper aims to extend our previous work on DEM simulations of concrete samples [25,26]. For completeness, this paper is, however, treated independently and therefore, a complete description of the DEM model is given. Note that the micro-mechanical model that is formulated here is a refined version of the one used in Refs. [25,26]. At the macro-scale (sample scale), the results of this study lay down the foundation for using the DEM to predict the response of concrete-like materials where stress reversals are involved. At the micro-scale, the findings from this and our previous works [25,26] provide a better understanding of the inter-particle interactions of such materials.

2. Multi-phase discrete element model

This section describes the multi-phase DE model used in this study. The term multi-phase indicates that distinction is made between different types of particles (aggregates and mortar) and the interactions that can exist between them (aggregate-mortar and mortar-mortar bonds). Characterizing aggregate-mortar and mortar-mortar bonds separately allows the interfacial transition zone (ITZ) to be taken into account, which is a major factor influencing the strength and behavior of concrete.

The overall mechanical properties of a particle assembly is the net result of the interactions between the assembly's individual particles. These interactions are categorized as either *contact* or *cohesive bond*. Contact interactions appear when two particles touch each other, while cohesive bond interactions are only created if two particles are in close proximity at the beginning of the analysis. From a simulation standpoint, the main difference between the two categories is that contact interactions can dynamically appear and disappear during an analysis, however, if an existing cohesive bond interaction breaks, it is permanently lost.

As mentioned before, this work uses a multi-phase implementation, which makes a distinction between aggregate particles and particles representing the mortar matrix [24,27]. Among the two, only mortar particles can form a cohesive bond with their neighbors. This is in contrast to single-phase models [28,29] where all particles are taken to be of the same material and all particles have the potential to form cohesive bonds. In the following text, properties associated with aggregate particles and mortar particles are distinguished by using the subscripts 'a' and 'm'.

2.1. Kinematics of cohesive bonds

As mentioned before, cohesive bonds are created only once, that is, at the start of the simulation. For a cohesive bond to exist between two particles, the two particles have to be in close proximity, and at least one of them has to be of mortar type. The spatial condition for a bond to exist between two particles i and j is:

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

where r_i and r_j are the radii of particles i and j, respectively, as illustrated in Fig. 1. The length of the distance vector $|\mathbf{d}_{ij}| = |\mathbf{x}_j - \mathbf{x}_i|$ is calculated from the center of particle i ($\mathbf{x}_i$) to the center of particle j ($\mathbf{x}_j$). In Eq. (1), $\gamma > 0$ is a parameter that allows a bond to be established when the two particles are in close proximity, but not