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Bonded-particle model calibration using response surface methodology

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ABSTRACT

The bonded-particle model (BPM) is commonly used in numerical analysis of the mechanical behavior of rock samples. Constructing a BPM model requires specification of a number of microstructural parameters, including the parallel-bond tensile strength, parallel-bond cohesion strength, parallel-bond effective modulus, parallel-bond friction angle, and parallel-bond stiffness ratio. These parameters cannot be easily measured in the laboratory or directly related to either measurable or physical material parameters. Hence, a calibration process is required to choose the values to be used in simulations of physical systems. In this study, response surface methodology along with the central composite design approach is used to calibrate BPMs. The sensitivities of the microparameters related to the uniaxial compressive strength (UCS) and elasticity modulus (i.e., the macroscopic responses of the models) are thoroughly scrutinized. Numerical simulations are performed to carefully assess the performance of the model. It is found that the elasticity modulus is highly correlated with the parallel-bond effective modulus. In addition, the parallel-bond tensile and cohesion strengths are the two most significant microparameters with a considerable effect on the UCS. The predicted values determined by the proposed approach are in good agreement with the observed values, which verifies the applicability of the proposed method.

Introduction

The discrete element method (DEM) or so-called distinct element method is regarded as an effective approach for engineering problems in granular and discontinuous materials. It has been widely used for granular flows, powder mechanics, rock mechanics, and comminution (Zhang, 2010). In addition, this method has been extensively used to simulate tumbling mills (Cleary, 1998; Cleary, Morrisson, & Morrell, 2003; Delaney, Cleary, Morrison, Cummins, & Loveday, 2013; Djordjevic, 2005; Khanal & Jayasundara, 2014; Mishra & Rajamani, 1992; Powell, Weerasekara, Cole, LaRoche, & Favier, 2011; Rajamani, Songfack, & Mishra, 2000; Wang, Yang, & Yu, 2012) and stirred mills (Plochberger & Avila, 2014; Sinnott, Cleary, & Morrison, 2006). A recent study has also verified the application of the DEM to comminution science (Cleary & Sinnott, 2015; Weerasekara et al., 2013).

The DEM is used to solve Newton's equations of motion, based on which particle motion can be effectively handled. Based on the contact law, the forces in interparticle contact can be determined (Weerasekara et al., 2013). Classical DEM simulations do not involve particle breakage, and hence they are most suitable for simulation studies of flow in non-breakable materials. This approach can also be applied to flows where the intensity of breakage can be determined from the energy spectrum. However, in some cases, such as the crushing chamber of crushers, it is essential to simulate the actual size reduction of particles in the flow of granular material. Because particles tend to move down in the crushing chamber, their size has to be reduced according to the applied forces (Herbst & Potapov, 2004). In the literature, there has been little tendency to simulate the crushing machine. This is mainly because of the following points: (a) to allow the particles to pass through the equipment, it is necessary to directly include breakage in the simulations, (b) it increases the number of particles in the crusher and thus results in a larger model size, and (c) it results to a high level of geometric complexity in the crusher (Cleary & Sinnott, 2015).

Different methods are used to model rock material breakage in the DEM. The population balance replacement model is the most commonly used approach. In this approach, if a load constraint is exceeded, a particle is replaced by a set of progeny particles. The size distribution of these particles is calibrated based on the breakage

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test data (Quist & Evertsson, 2016). Potyondy and Cundall (2004) proposed the bonded-particle model (BPM). This approach uses imaginary beams among the contacted particles to bond a cluster of subparticles. A third approach applies tetrahedral mesh elements to model a specific particle. In this approach, compliant contacts and stress constraints are considered in both the normal and tensile directions.

A recent report by Lisjak and Grasselli (2014) provides a complete review of the different approaches used to model breaking of rock particles. For instance, Herbst and Potapov (2004) and Quist and Evertsson (2010) focused on developing models for lab-scale cone crushers. Single particle breakage in jaw crushers was investigated by Refahi, Mohandesi, and Rezai (2010). It should be mentioned that all of the mentioned approaches are based on BPMs. A method has been developed to model discrete grain breakage (Herbst & Potapov, 2004). The method treats the crusher based on a bonded sphere model including bonded tetrahedral elements. Lichter, Lim, Potapov, and Kaja (2009) introduced the fast breakage model. This approach uses polygonal elements to include DEM particles. Following a fracture event, particle replacement of the breakage progeny is realized based on a microscale population balance model (Lisjak & Grasselli, 2014).

The BPM has been used to investigate the mechanical behavior of rocks (Cundall & Strack, 1979; Ivars et al., 2011; Kulatilake, Malama, & Wang, 2001; Potyondy & Cundall, 2004) and characterize the breakage properties of rocks in milling or crushing (Refahi et al., 2010; Whittles, Kingman, Lowndes, & Jackson, 2006). The same approach was also used to investigate rail ballast (Thakur, Vinod, & Indraratna, 2010), where the authors used the particle-flow code in two-dimensions with simple breakage models. Using a similar approach, Estay and Chiang (2013) proposed application of the particle-flow code in three-dimensions. It is well-known that each collection of grains that is joined by cement shows specific mechanical behavior. The BPM replicates such behavior in rock (Weerasekara et al., 2013). Similar approaches, such as the Rumpf model (Laitinen, Bauer, Niinimäki, & Peuker, 2013; Rumpf, 1990; Sigmund, El-Shall, Shah, & Moudgil, 2008), are available in other research fields. These models can also include structural properties such as the bond strength and bond cross-sectional area to represent the aggregate strength.

The basic concept of the traditional BPM is to represent the rock as densely packed disks or spheres that are bonded together at their contacts, and then simulate its mechanical behavior. If an adequate control action is performed on the strength and mechanical properties of the bonds, it results in similar behavior to that of the mechanical properties of the rock material (Weerasekara et al., 2013). The mechanical behavior of a BPM specimen is described by the movement of each particle along with the forces and moments acting at each contact between two constitutive particles (Ding & Zhang, 2014).

The bond is represented by a thin finite area plate (Fig. 1(a)) and includes five parameters: the normal and shear stiffnesses per unit area $\overline{k_n}$ and $\overline{k_s}$, the tensile and shear strengths σ_c and τ_c, and the bond-radius multiplier, $\overline{\lambda}$, which defines the bond radius $\overline{R} = \overline{\lambda}\min(R_A, R_B)$, with R_A and R_B being the radii of the bonded particles. The relative motions between the two contact particles cause changes in the contact forces and moments owing to the contact stiffness. The forces and moments acting at the contact are shown in Fig. 1(b).

The particle movements and the resultant forces and moments follow Newton's law of motion. The change of the contact forces and moments owing to the relative particle movements are determined by

$$\Delta\overline{F_n} = -\overline{k_n}A\Delta d_n, \quad \Delta\overline{F_s} = -\overline{k_s}A\Delta d_s, \tag{1}$$

$$\begin{cases} \Delta\overline{k_n} = -\overline{k_s}J\Delta\theta_n \\ \Delta\overline{M_s} = -\overline{k_n}I\Delta\theta_s \end{cases}, \tag{2}$$

where $\overline{F_n}$, $\overline{F_s}$, and $\overline{M_n}$, $\overline{M_s}$ are the contact forces and moments at the center of the contact zone, respectively, in the normal (n) and shear (s) directions, d_n, d_s and θ_n, θ_s are the relative displacements and rotations between the two bonded particles, respectively, in the normal (n) and shear (s) directions; and A, I, and J are the area, moment of inertia, and polar moment of inertia of the bond cross-section, determined by (Ding & Zhang, 2014; Potyondy & Cundall, 2004)

$$A = \pi\overline{R}^2, I = \frac{1}{4}\pi\overline{R}^4, J = \frac{1}{2}\pi\overline{R}^4. \tag{3}$$

The maximum tensile and shear stresses, $\overline{\sigma}_{max}$ and $\overline{\tau}_{max}$, acting at the contact are obtained by (Ding & Zhang, 2014)

$$\overline{\sigma}_{max} = \frac{\overline{F_n}}{A} + \frac{\overline{M_s}\overline{R}}{I}, \tag{4}$$

$$\overline{\tau}_{max} = \frac{\overline{F_s}}{A} + \frac{\overline{k_n}}{\overline{R}}J. \tag{5}$$

If $\overline{\sigma}_{max} \geq \overline{\sigma}_c$ or $\overline{\tau}_{max} \geq \overline{\tau}_c$, the bond breaks by tension or shear and the bond along with its forces, moments, and stiffness is then removed from the particle (Ding & Zhang, 2014).

In DEM analysis, it is crucial to select appropriate parameters for accurate simulation of real and physical systems (Hanley, O'Sullivan, Oliveira, Cronin, & Byrne, 2011). For numerical simulations using DEM implemented in the particle-flow code (PFC), the macroscale mechanical properties of the rock cannot be directly included in the model. Only microscale mechanical parameters are specified for the particle assembly that hypothetically represents the actual rock material (Wang, Xu, Li, Liu, & Peng, 2013). A higher confidence degree is attained in estimating/measuring the input parameters, namely, the particle dimensions or their density. However, experimental studies fail to identify the rheological parameters as inputs for contact constitutive models (Hanley et al., 2011). Therefore, a calibration approach is often used to select these parameters. Typically, calibration involves varying the DEM parameters until the model response closely corresponds to the equivalent physical experimental response. While conceptually simple, this calibration approach has many drawbacks: it may take several trial tests and a long time to obtain an appropriate set of parameters, it is impossible to know how many DEM simulations are required for calibration in advance, the final parameters obtained may not be optimal, and the mechanistic insight gained is limited (Hanley et al., 2011).

In the calibration process, two main steps need to be performed. The first step is parameter identification (Wang & Tonon, 2009), which relates the microparameters to the macromaterial properties. The second step is called parameter quantification, which assigns the parameters certain values to reproduce the experimental behavior of the testing material. Parameter identification of the BPM has been discussed by Potyondy and Cundall (2004). The framework of this method is shown in Fig. 2. Uniaxial compression tests are simulated and then compared (steps 1 and 2). Hsieh, Li, Huang, and Jeng (2008) proposed a similar concept, where uniaxial compression is firstly modeled using the BPM and it is iteratively revised until it gives reasonable macroscopic uniaxial compression behavior (similar uniaxial compressive strength (UCS) and Young's modulus). This test also determines the BPM microscopic parameters (Hsieh et al., 2008). The only approach to allocate the microparameters of the PFC model is the "trial and error" method. However, it is a primitive method aligned with a high computational burden. Only a few attempts have been made to improve and

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