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A new contact model to improve the simulated ratio of unconfined compressive strength to tensile strength in bonded particle models

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ABSTRACT

The bonded particle model (BPM) has been increasingly used to simulate and analyze the mechanical behavior of rocks. However, traditional BPMs that use symmetric particles bear the intrinsic limitation of severely overestimating the tensile strength of simulated rock and leading to unrealistically low unconfined compressive strength to tensile strength (*UCS*/*T*) ratio. Researchers have proposed different methods to increase the *UCS*/*T* ratio in BPM simulations; but they all have limitations. In this paper, a new contact model which properly considers the contribution of moments to normal and shear contact stresses and the condition at which the contact fails was proposed and implemented in the three-dimensional Particle Flow Code (PFC3D). The new contact model does not impose significant additional calculation burden. Detailed parametric studies were performed to evaluate the effect of different microscopic parameters on the *UCS*/*T* ratio of BPM specimens. The results indicate that the moment contribution, cohesion and tensile strength are three key factors affecting the *UCS*/*T* ratio. When the value of the moment contribution parameters is smaller than 0.5, a wide range of *UCS*/*T* ratios can be achieved by changing the cohesion and/or tensile strength values. Finally, the new contact model was used to simulate two widely studied rocks, Lac Du Bonnet (LDB) granite and Carrara marble, and the obtained *UCS*/*T* ratios were in good agreement with the measured values from laboratory experiments.

1. Introduction

The bonded particle model (BPM) has been used by many researchers to study the mechanical behavior of rocks [1–13]. The basic idea of traditional BPM is to represent rock as a material of densely packed disks or spheres that are bonded together at their contacts and then simulate its mechanical behavior. BPMs can be used to simulate complex mechanical behavior of rocks by using appropriate microscopic parameters for the particles and contacts. However, it is found that simulations BPMs tend to overestimate the tensile strength when the compressive strength is matched, and lead to unrealistically low ratios of unconfined compressive strength to tensile strength (*UCS*/*T*) [6,14]. The *UCS*/*T* ratio is an important property of rock related to its fundamental characteristics [15]. Although *UCS* is the most widely used parameter to characterize rock in engineering practice, it is now well known that the brittle failure of rock is dominated by tensile rupture [16–18]. The unrealistically high tensile strength from BPM simulations may lead to false prediction of crack initiation and propagation in rock. Therefore, the limitation of low *UCS*/*T* ratio restricts the capability of BPM to simulate problems where the stress path may be either compression or tension.

This paper studies the basic mechanism that leads to the significantly underestimated *UCS*/*T* ratio from BPM simulations, reviews the different methods proposed by researchers to increase the *UCS*/*T* ratio, and finally develops a new contact model so that the correct *UCS*/*T* ratio can be obtained. The developed new contact model was successfully implemented in the widely used three-dimensional BPM software Particle Flow Code (PFC3D) [2,3].

2. Literature review and discussion

Different BPMs have been proposed in the literature to simulate the mechanical behavior of intact rock [1,19]. However, regardless of he predefined microscopic parameter values are used, they all tend to significantly over predict the tensile strength after the compressive strength is matched, and thus lead to a *UCS*/*T* ratio much smaller than the laboratory test values. Typically the test *UCS*/*T* values are between 10 and 20 for intact rock, but the BPMs give *UCS*/*T* ratios of 3 to 7 [1,6,14,19]. LDB granite is one of the well-simulated rocks using two-dimensional BPM software PFC2D [1,4] and three-dimensional BPM software PFC3D [1,14]. As Potyondy and Cundall [1] and Schopfer et al. [14] have mentioned,

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BPMs have difficulty in reproducing the laboratory *UCS*/*T* value for LDB granite. According to the micro-scale failure behavior analysis [18,20–24], the reasons for the low *UCS*/*T* ratio from BPM simulations are: (1) the symmetrical particles used in simulations cannot properly reproduce the particle interlocking and rotational resistance behavior of rock grains; and (2) the dominant tensile failure in both the uniaxial compression and direct tension tests indicates that both the *UCS* and *T* are determined by the bond tensile strength. Researchers have attempted different methods to tackle this problem [1,6,14,23,24]. These methods can be divided into three categories: (1) modifying particle texture such as using clump and cluster particles, (2) modifying contact bond condition such as partial release of contacts, and (3) modifying the contact model such as eliminating the contribution of moments to contact stresses. These methods are briefly discussed below

The first category of methods imposes additional texture to the symmetrical particles in order to increase particle interlocking and friction resistance. The particle interlocking contributes to high internal friction angle and thus high *UCS*/*T* ratio. Indeed, the mechanical behavior of rock relies on its microstructure and combination of mechanisms occurring at the grain scale [25]. Boutt and McPherson [26] used PFC2D to investigate the effect of particle packing and particle shape on the macroproperties of PFC specimens and concluded that particle packing is an important factor affecting the mechanical behavior of simulated specimens. Based on the analysis of a combined finite-discrete element method model, Xiang et al. [27] indicated that the non-spherical geometry and wide particle size distribution are of crucial importance in affecting the mechanical behavior of the particulate system. The utilization of polygonal particles to replicate the microstructure and simulate the macroscopic behavior of rocks with other two dimensional codes by Kazerani and Zhao [28] and Lan et al. [29] also shows the importantce of particle shape in afecting the mechanical properties of simulated rocks. Using PFC2D, several researchers tried to increase the *UCS*/*T* ratio by generating irregularly shaped discrete elements such as clumps proposed by Itasca [3] and Potyondy and Cundall [2], clusters by Cho et al. [24] and approximate polygon particles by Potyondy [22]. The results indicate that these methods can effectively increase the particle interlocking and thus increase the *UCS*/*T* ratio from PFC2D simulations. When utilized in PFC3D, however, these methods have the problems not only in the significantly increased calculation time, but also in the effectiveness to increase the *UCS*/*T* ratio. Ding and Zhang [6] reported that even after 50% of the regular spherical particles are replaced by clump particles, only a slight increase of the *UCS*/*T* ratio (still smaller than 10) can be achieved in PFC3D simulations. To effectively increase the *UCS*/*T* ratio in PFC3D simulations, prisms and other more complex-shaped particles should be used. However, the utilization of complex-shaped particles may introduce heterogeneity, anisotropy and scale effects and make it more difficult to develop a correlation between the simulations and the physical materials [30].

The second category of methods modifies the contact bond condition, including partial release of contacts [6,14] and increase of bond density by enlarging the interaction range [20]. The release of contacts is a direct imitation of pre-existing micro cracks in rock and helps generate particle interlocking as the unbonded particles start to move at an earlier stage and sliding occurs at the rugged unbonded surface. The unbonded contacts do not bear tensile or shear strength but will yield frictional resistance during sliding under compression. This feature indicates that the unbonded contacts can bear some load in compression but not in tension and thus the *UCS*/*T* ratio increases with a greater percentage of unbonded contacts. Ding and Zhang [6] indicated that the *UCS*/*T* ratio can be doubled when 50% of contacts are released in PFC3D but still is not large enough compared to the *UCS*/*T* ratio from experiments. The adjustment of particle microstructure to increase particle interlocking can also be achieved by increasing the bond density between particles [20,31–33]. The method to increase the bond density via manually increasing the bond interaction range has been proven effective in increasing the *UCS*/*T* ratio to over 20 [20,34]. However, the problems similar to those in the methods of the first category will arise. For example, more complexity can be added to the calibration of the microscopic parameters to the physical material properties.

The third category of methods modifies the constitutive contact model to reach higher *UCS*/*T* ratio. The mechanical behavior of a material is simulated in BPM by associating a constitutive model with each contact of particles. A contact model describes the force-displacement response at a contact and the condition at which the contact fails. During each calculation cycle, the BPM code calls the contact model and the forces and moments acting at the contact are updated. By default, BPM uses disks in 2D and spheres in 3D as the discrete element particles. This simplification ensures calculation efficiency and reduced number of microscopic parameters to categorize the material behavior. The rotational resistance at the contact is considered as bending and twisting (only in 3D) moments in the default parallel-bond model [3]. The maximum normal and shear stresses carried by the contact are affected by the accumulation of bending and twisting moments. Aspired by the failure behavior of grain based model [22], Potyondy [23] modified the default contact model in PFC to eliminate the contribution of moments to the maximum normal and shear stresses on the contact. By completely ignoring the stresses caused by the bending and twisting moments, he successfully reached the measured *UCS*/*T* ratio of Äspo diorite. The complete elimination of moment contribution to the maximum stresses at the contact results in smaller displacement and rotation undertaken by the bond and thus postpones the breakage of the bond. In other words, the bond is strengthened. However, the stresses from the bending and twisting response do exist and are carried by the contact as the bond moments. The importance of rotational inertia and energy loss in the rotation of particles has been emphasized in both physical experiments [35–38] and numerical studies [39–41]. The rotational resistance is often referred to as rolling resistance or rolling friction [42]. The rolling resistance is important regarding the interlocking of particles. Bardet and Huang [39] introduced rotational constraints into a DEM model when simulating the micropolar effects in an idealized granular material. They and later researchers [43,44] demonstrated that the overall internal friction angle of a particle assembly is higher when the particle rotation is fixed than that when the particles are free to rotate. A more realistic contact model should properly consider how the bond resists relative particle rotation. Potyondy proposed another modified contact model called flat-jointed model in two dimensions [45,46] and then extended it to three dimensions [47]. The flat-jointed model mimics the polygonal grain structure in natural rock by using a notional finite length (2D) or area (3D) flat surface at each particle contact. The flat joint interface is segmented, with each segment initially bonded or unbonded. As the bonded segments break, the interface changes from fully bonded state to partially bonded state and then fully unbonded and frictional state. During this process, the flat joint is not removed and thus a fully broken interface continues to resist relative rotation. With carefully calibrated tensile and cohesive bonding strengths, the correct *UCS*/*T* ratio of Äspo diorite was successfully matched using this model. The imaginary flat joint interface imposes particle interlocking and friction resistance at the contact and restricts the relative movement of particles. The segmented flat interfaces also increase computational burden compared to the conventional bonded-particle model.