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Effects of model size and particle size on the response of sea-ice samples created with a hexagonal-close-packing pattern in discrete-element method simulations

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ABSTRACT

We investigated the effects of model size and particle size on the simulated macroscopic mechanical properties, uniaxial compressive strength, Young's modulus, and flexural strength of sea-ice samples, using the discrete-element method (DEM) with a bonded-particle model. Many different samples with a hexagonal-close-packing pattern and a unique particle size were considered, and several ratios of particle size to sample dimension (D/L) were studied for each sample. The macroscopic mechanical properties simulated by the DEM decrease monotonously with an increase in D/L. For different samples with different particle sizes, the macroscopic mechanical properties will be identical when D/L is constant. The quantitative relationships between macroscopic mechanical properties and ratio of particle size to sample size are important aspects in engineering applications of the DEM method. The results provide guidance on the choice of a particle size in the DEM simulation for numerical samples with a hexagonal-close-packing pattern.

Introduction

Since Potyondy and Cundall (2004) first proposed the discrete-element method (DEM) with a bonded-particle model for geo-mechanics applications, which they termed the BPM, the BPM method has proven to be a very powerful and versatile numerical method to simulate the crushing behavior of brittle materials, such as rock, concrete, and sea ice. Unlike continuum methods that use average measures of material degradation in constitutive models to represent microscopic damage, the discontinuum BPM idealizes material as a collection of separate particles that are bonded together at contact points and uses bond breakage to represent damage (Potyondy & Cundall, 2004). The assignment of microscopic model parameters is an important aspect, either in engineering applications of the BPM method or the mechanical mechanistic studies of materials. The microscopic model parameters cannot be determined directly through theoretical analysis or be measured during mechanical experiments. The common method that is used to carry out a numerical calibration is to back-calculate the microscopic parameters. The microscopic model parameters are determined through an iterative trial–error process by conducting a series of numerical simulations of fundamental mechanical tests, e.g., uniaxial compressive tests and three-point bending tests. The uniaxial compressive tests were used to reproduce the deformability behavior and the uniaxial compressive strength, three-point bending tests were used to reproduce the flexural strength, until the microscopic model parameters reproduce or approximate the measured macroscopic mechanical properties (Ding, Zhang, Zhu, & Zhang, 2014). It is still difficult to reproduce all complicated behaviors by calibrating the BPM model.

Huang (1999) investigated the relationships between microscopic model parameters and macroscopic mechanical properties of two-dimensional samples using PFC2D software. In general, the set of model parameters that influences the macroscopic properties of the material is $\left\{L, D, \rho, n, k^{\mathrm{n}}, k^{\mathrm{s}}, \mu, \sigma_{\mathrm{b}}^{\mathrm{n}}, \sigma_{\mathrm{b}}^{\mathrm{s}}, v_{\mathrm{L}}\right\}$, where L is the sample size (the value here is used to illustrate the influencing factor, and does not refer to a certain size); D is the particle size; ρ is the material density; n is the porosity of the DEM numerical sample; k^{n} and k^{s} are the normal and tangential contact stiffness, respectively; $\sigma_{\mathrm{b}}^{\mathrm{n}}$ and $\sigma_{\mathrm{b}}^{\mathrm{s}}$ are the normal and tangential interparticle bonding strength, respectively; and μ is the friction coefficient between two particles. The parameters L and ρ can be obtained directly from the sample properties. According to the Buckingham π theorem, six independent dimensionless parame-

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ters that govern the macroscopic properties of a sample are given by $\left\{D/L, k^s/k^n, \mu, n, \sigma_b^s/\sigma_b^n, \upsilon_L/\sqrt{k^n/\rho}\right\}$. $\sqrt{k^n/\rho}$ is dependent on the speed of the compressive wave that propagates in an elastic medium. The loading velocity is small compared with the speed of the elastic wave, and it can maintain a quasi-static loading. The parameter $\upsilon_L/\sqrt{k^n/\rho}$ is no longer considered in the expression above.

Many researchers have investigated the calibration of microscopic model parameters and tried to establish the relationships between microscopic model parameters and macroscopic mechanical properties. It is thought that the microscopic elastic parameters, k^n and k^s/k^n, will influence the macroscopic elastic properties: Young's modulus E and Poisson's ratio υ (Huang, 1999; Wang & Tonon, 2010; Yang, Jiao, & Lei, 2006). These studies have shown that Young's modulus increases linearly with increasing contact normal stiffness. Poisson's ratio decreases nonlinearly, with an increasing ratio of shear to normal contact stiffness k^s/k^n. The analytical solution of E and υ can be obtained for samples in which spherical particles are arranged in a hexagonal-close-packing (HCP) lattice (Wang & Alonso-Marroquin, 2009). The microscopic strength parameters, σ_b^n, σ_b^s/σ_b^n, and μ will influence the macroscopic strength properties (Ji, Di, & Long, 2016; Schöpfer, Childs, & Walsh, 2007). The effects of interparticle contact stiffness and bonding strength on the macroscopic deformability and strength are intuitive and easy to obtain. The deformability and strength properties will not be considered in detail, and more attention will be focused on the effect of sample size and particle size.

Many studies have indicated that the sample size and particle size are important factors to consider in each numerical simulation (Ding et al., 2014; Schöpfer et al., 2007). Ding et al. (2014) summarized some sets of model parameters used in separate DEM numerical simulations implemented on PFC2D or PFC3D, in which samples were tested with random packing patterns and the particle sizes ranged from a minimum particle diameter d_{min} to a maximum particle diameter d_{max}. These results showed some fluctuation of simulated macroscopic properties with the D/L ratio, where D is the particle size and L is the sample size. Some common relationships between macroscopic mechanical properties and particle and model size have been obtained by a sensitivity analysis, that is, the uniaxial compressive strength and Young's modulus decrease with an increasing ratio of D/L, and the Poisson's ratio increases with an increasing ratio of D/L (Ding et al., 2014; Yang et al., 2006). Besides spherical particles, similar issues on the elemental size effect have been investigated using polygonal blocks (Yao, Jiang, & Shao, 2015).

In an investigation of the relationship between microscopic model parameters and macroscopic mechanical properties, random packing patterns and various particle size distributions are used frequently to implement different DEM simulations (Ding et al., 2014; Huang, Hanley, O'Sullivan, & Kwok, 2014; Nitka & Tejchman, 2015; Potyondy & Cundall, 2004; Schöpfer et al., 2007; Yang et al., 2006). Relevant research work on the regular packing of samples is uncommon. We have used a sample with a regular packing pattern and a unique particle size to establish quantitative expressions to guide the engineering application of the BPM model. We have studied the effect of sample size and particle size on the DEM simulation results.

Failure criteria of bonded particles in DEM

The sea ice is discretized into a set of spherical particles that are attached using a parallel bond model, as shown in Fig. 1. A linear elastic force–displacement contact model was used, and the ice particles are either bonded or de bonded with a linear elastic material with the mechanical properties of sea ice. A parallel bond can be described by the following five parameters: normal and shear stiffness, k^n and k^s, respectively (N/m); normal and shear strength, σ_b^n and σ_b^s, respectively (MPa); and bonding disk radius, R. Normally, R is set as the smaller radius of the two bonded particles (Potyondy & Cundall, 2004) or their mean radius (Nitka & Tejchman, 2015; Wang & Tonon, 2009). In this study, the disk radius R is set at the same value as the two bonded particles. The force and moment that are carried by the parallel bond can be resolved into normal and shear components as $\mathbf{F}_n$, $\mathbf{F}_s$, $\mathbf{M}_n$, and $\mathbf{M}_s$. The maximum tensile and shear stresses that act on the parallel-bond periphery are calculated based on beam theory as (Potyondy & Cundall, 2004):

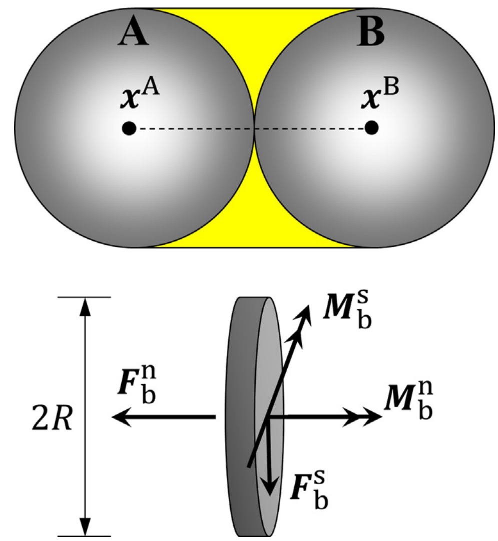

Fig. 1. Bonding model between two spherical particles.

$$\sigma_{max} = \frac{-|\mathbf{F}_n|}{A} + \frac{|\mathbf{M}_s|}{I}R, \ \tau_{max} = \frac{|\mathbf{F}_s|}{A} + \frac{|\mathbf{M}_n|}{J}R, \tag{1}$$

where A, I, and J are the area, moment of inertia, and polar moment of inertia of the parallel bond, respectively. These quantities are given by:

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

If the maximum tensile stress exceeds the normal strength ($\sigma_{max} > \sigma_b^n$), or the maximum shear stress exceeds the shear strength ($\tau_{max} > \sigma_b^s$), then the parallel bond breaks. The parallel bond is removed from the contact model, and the two particles that are associated with this parallel bond will make contact as separate particles.

Sea ice was treated as a type of rock-like material with elastic–brittle properties. In the failure criterion, for tensile failure, an elastic brittle behavior is characterized by a tensile strength σ_b^n for all bonds between adjacent particles. Once the tensile stress in the bond reaches the tensile strength σ_b^n, the tensile and shear stresses reduce to zero instantaneously. For shear failure, a Mohr–Column criterion is used to define the bond shear strength. The shear strength is defined by using the coefficient μ_b and is determined as:

$$\tau_b = \sigma_b^s + \mu_b \sigma^n, \tag{3}$$

where τ_b is the shear-strength envelope between bonded particles under the influence of normal stress, σ_b^s is the interparticle shear bonding strength, and σ^n is the normal compressive stress. The shear failure criterion is illustrated by Ji et al. (2016). A preliminary investigation indicated that the mechanical strengthof sea ice is dependent on the coefficient μ_b (Ji et al., 2016). Specifically, the ratio of compressive to flexural strength of sea ice increaes with an increase of this coefficient.