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Incorporating surface roughness into DEM models of crushable soils

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1 INTRODUCTION

One obvious characteristic of granular grains is that their surface is not smooth, especially when observed at smaller scales. Some advanced experiment imaging methods such as optical interferometry, scanning electron microscopy and atomic force microscopy have been developed and successfully used to characterize and quantify grain surface roughness. One fundamental finding is that surface roughness can significantly affect mechanical behavior of granular materials.

Grain crushing is of importance for several geotechnical problems, such as side friction on driven piles, railway ballast durability and slaking induced irreversible deformations. Discrete Element Method (DEM) has been widely used to model grain crushing and has gained wide acceptance with its own advantages in providing micro-scale mechanical observations of granular materials (Zhou et al. 2019). However, in those models of breakable grains, grain surface roughness effects were rarely included, leading to a certain misuse of contact parameters (Ciantia et al. 2019).

In this paper, a well-established DEM crushing contact model and a rough Hertzian contact model are combined to incorporate both effects in a single contact model. The paper is organized as follows. First, a brief introduction of the rough-particle crushing model is proposed. Then a simple particle failure test is conducted to validate the correct implementation of the rough model.

2 DESCRIPTION OF ROUGH-PARTICLE CRUSHING MODEL

The rough contact model proposed by Otsubo et al. (2017) was chosen to describe grain surface roughness (S_q) effect. It is created on the basis of Hertzian contact model. In this model, the relationship between normal contact force (F_n) and displacement (δ) is composed by three phases: asperity-dominated, transitional and Hertzian (Fig. 1). Two model parameters δ_1 and δ_2 are defined to control the overall F_n-δ relationship. In terms of the coordinates of the two separation points, δ_{T1} and δ_{T2} are threshold contact displacements that correspond to a contact force equal to F_{nT1} and F_{nT2} respectively.

A particle crushes once its limit maximum force F_{lim} is reached. Based on the work of Russell & Muir Wood (2009), a two-parameter material strength criterion was used (Ciantia et al. 2015)

$$F_n \leq F_{lim} = \sigma_{lim} A_F \;\; \Rightarrow \;\; F_n \leq \sigma_{lim,0} f(var) \left(\frac{d}{d_0}\right)^{-\frac{3}{m}} \pi r' \delta \qquad (1)$$

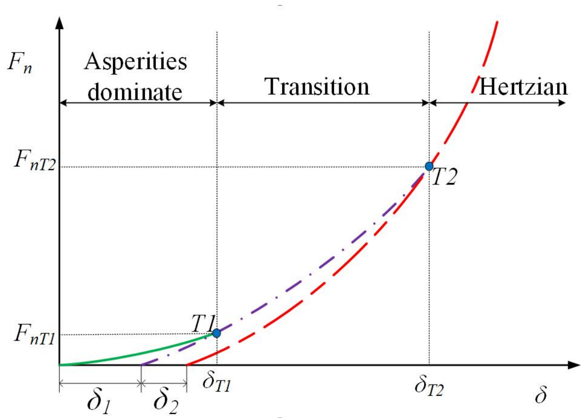

Figure 1. Rough contact model composed by three stages (Otsubo et al. 2017).

Where σ_{lim} is the limit strength of the material and A_F is the contact area. Affected by large natural variabilities in shape, microstructure and contact conditions, the limit strengths differ for particles with the same size. *f(var)* is a function used to incorporate the natural material variability into the model, where the limit strength, σ_{lim} is assumed to be normally distributed for a given sphere size. The coefficient of variation of the distribution, *var*, is taken to be a material parameter. The mean strength value ($\sigma_{lim,0}$) depends on the particle diameter (*d*) where *m* is a material constant, d_0 is the reference diameter. δ is the contact overlap between two spheres. If Hertzian contact theory is used to calculate contact area, δ can be expressed as

$$\delta = \left(\frac{9F_n^2}{16r'E'^2}\right)^{\frac{1}{3}} \tag{2}$$

Where, *E'* and *r'* are given by

$$E' = \left(\frac{1-v_1^2}{E_1} + \frac{1-v_2^2}{E_2}\right)^{-1} \tag{3}$$

$$r' = \left(\frac{1}{r_1} + \frac{1}{r_2}\right)^{-1} \tag{4}$$

The subscripts '1' and '2' refer to the two contacting particles. E_i, v_i and r_i are the Young's modulus, the Poisson's ratio and the radius of particle *i*, respectively. On the other hand, when the rough contact model is employed, contact overlap expression has three different forms corresponding to each phase. Hence the rough-particle crushing criteria is expressed as

$$F_n \leq F_{lim} = \sigma_{lim,0} f(var) \left(\frac{d}{d_0}\right)^{-\frac{3}{m}} \pi r' \left(\frac{F_n}{S_q E' \sqrt{2r'S_q}}\right)^{\frac{1}{c}} \left[\left(\frac{1}{100}\right)^{\frac{1}{b}} \left(5\sqrt[3]{90}S_q + n_2 S_q\right) + n_1 S_q\right]$$

When, $F_n \leq F_{nT1}$ (5)

$$F_n \leq F_{lim} = \sigma_{lim,0} f(var) \left(\frac{d}{d_0}\right)^{-\frac{3}{m}} \pi r' \left[\left(\frac{F_n}{100 S_q E' \sqrt{2r'S_q}}\right)^{\frac{1}{b}} \left(5\sqrt[3]{90}S_q + n_2 S_q\right) + n_1 S_q\right]$$

When, $F_{nT1} \leq F_n \leq F_{nT2}$ (6)

$$F_n \leq F_{lim} = \sigma_{lim,0} f(var) \left(\frac{d}{d_0}\right)^{-\frac{3}{m}} \pi r' \left[\left(\frac{9F_n^2}{16E'^2 r'}\right)^{\frac{1}{3}} + n_1 S_q + n_2 S_q\right]$$

And when, $F_{nT2} \leq F_n$ (7)

while b and c are constants that depend on the two model parameters δ_1 and δ_2. $\delta_1 = n_1 S_q$ and $\delta_2 = n_2 S_q$ where n_1 and n_2 are model parameters coefficients. Detailed expressions used to calculate F_{nT1}, F_{nT2}, δ_{T1}, δ_{T2}, b and c are listed in Otsubo et al. (2017). Once the limit condition is reached, the spherical particle is split into smaller inscribed tangent spheres. The crushed fragments assume the velocity and material parameters of the original particle. Ciantia et al (2015) concluded that a 14-ball crushed configuration can adequately represent macroscopic behavior.

The contact model presented above was implemented in *PFC3D* (Itasca 2017) by means of a C++ coded user defined contact model (UDCM). Generally, functions coded into UDCM can execute much faster than the equivalent *FISH* functions. The original implementation (Ciantia et al. 2015) required a *FISH* coded time-consuming loop through all the contacts that is not required in the UDCM. In the current version, all particles that meet the failure criterion are recorded by looping through all the contacts during one step. A *FISH* function then performs the 14-ball replacement for these particles. The computational efficiency of UDCM in detecting breakage in particles with Hertzian model without roughness has been validated by Ciantia et al. (2017).

3 VALIDATION OF CORRECT IMPLEMENTATION

To validate the correct implementation of the rough contact model and the crushing model through UDCM, preliminary results derived from the UDCM are illustrated in Figure 2. They are compared with analytical expressions for ball-ball contact. The parameters adopted are listed in Table 1, where G is the shear modulus. To test ball-ball contacts, the compression of two spheres is modelled. F_1, F_2 and F_3 represent contact forces in asperity-dominated, transition and Hertzian phases, respectively. A good agreement can be seen for results from both numerical and analytical frameworks for particle crushing (Fig. 2a). Figure 2b illustrates the evolution of F_n- δ curve for crushable particles with ($S_q = 1$ μm) and without ($S_q = 0$ μm) roughness. It can be observed that before crushing occurs, at a specific contact force, the model with roughness produces larger overlap than the one without roughness, meanwhile the gap increases with the increase of F_n. The presence of surface roughness causes an increase of particle crushing force.

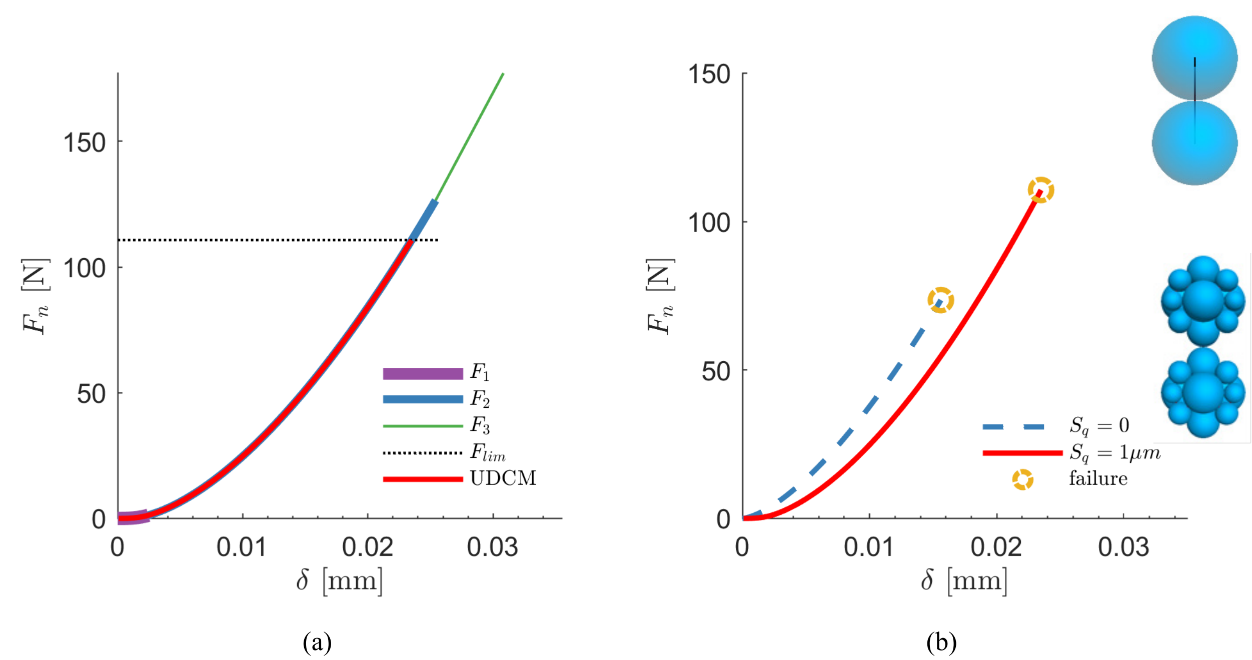

Figure 2. Single-grain platen test.

Table 1. Parameters used for UDCM validation.

Parameters	d_0/mm	d/mm	G/GPa	v	φ	m	$\sigma_{lim,0}$ /GPa	S_q/μm	n_1	n_2
Values	2	2	32	0.2	0.275	7.5	3	1.0	1	2

4 CONCLUSIONS

In this work, a rough-particle crushing criteria is successfully developed by combining the rough Hertzian contact model and the DEM crushing model. The model is implemented through into *PFC3D* the way of user defined contact model. Its correct implementation is validated by testing ball-ball contacts. Further work is expected to improve the reliability of DEM simulations of granular materials by using more realistic contact parameters.

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