Proceedings of the 24th UK Conference of the
Association for Computational Mechanics in Engineering
31 March – 01 April 2016, Cardiff University, Cardiff

Random Normal Contact Laws for Particles with Rough Surface in Discrete Element Modelling

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ABSTRACT

Particles are assumed smooth in classical discrete element modelling, but real particles have random rough surfaces which may influence their mechanical properties. It is necessary therefore to quantitatively improve the conventional discrete element model by taking the surface roughness into consideration. In this work, a new normal contact law is established for particles that have random rough surfaces. The contact law, based on the classic Greenwood and Williamson (GW) model, is derived by both theoretical derivation and numerical calculations. Instead of a complicated integral expression involved in the GW model, the resulting empirical formula of the law retains the closed form and simplicity of the Hertz model, with only one added parameter, σ_s, the standard derivation of a surface roughness, and therefore can be readily incorporated into the current discrete element modelling framework.

Keywords: *Surface roughness; Contact law; Discrete element method, Stochastic DEM; Numerical model*

1. Introduction

The discrete element method (DEM) is a computational technique originally developed by Cundall and Strack [3] which is well suited to simulate the response of assembly systems of particles [9]. DEM has been widely accepted as an effective method to model engineering problems in granular and discontinuous materials, especially in granular flows, power mechanics and rock mechanics. The basic particles in DEM are regular geometric entities such as disk, sphere, ellipse and ellipsoid with smooth surface. However real particles contain geometric irregularities at both macroscopic and microscopic levels. The macroscopic irregularities of particles may be modelled by more complicated geometric shapes, while surface irregularities at the microscopic level, also called the surface roughness, are more difficult to be considered, although they may have strong influence on the phenomena of contact, friction, wear and lubrication [1]. Up to now, very few attempts have been reported to provide random interaction laws that can be readily applied in DEM to estimate the contact forces between rough particles. It is therefore necessary to quantitatively improve the classical DEM by taking the surface roughness into consideration. The main objective of this paper is to establish a new random interaction law which can be applied in DEM for particles having random rough surfaces.

There are several approaches that have been developed to understand the contact mechanism between rough surfaces, and can be classified into two categories: statistical and deterministic. The earliest and most recognized statistical treatment of rough surfaces is the work of Greenwood and Williamson [6]. This method can be viewed as a single scale method since statistical parameters used to represent rough surfaces are scale-dependent. Another statistical approach, where a fractal curve/surface is adopted to describe a rough surfaces together with a contact mechanism to resolve the contact, is introduced by Majumdar and bhushan [8]. This fractal based approach can be regarded as multiple scaled because of the inherent multi-scale invariant characteristics of most fractal curves/surfaces. On the other hand, the deterministic methods attempt to model rough surfaces precisely and the resulting contact problem is typically solved by the finite element method. Furthermore, the fast Fourier transformation is often used to treat the rough surface [10]. For the contact between two rough curved bodies, the first analytical study was conducted by Greenwood and Tripp [5] who employed the GW asperity contact model together with the bulk surface deformation for circular point contact. More recent researches have extended the GW approach to the elasto-plastic deformation regime [2, 4, 7].

2. Numerical algorithms for the GW model

In the GW model, a rough flat surface is assumed to be an assembly of asperities whose properties are obtained from a given statistical height distribution of the surface and the Hertz contact law is then applied to these asperities which are also assumed to have the same radius of curvature. When this theory is applied to the contact problem of two rough spheres [6], the only difference from the rough flat contact problem is the geometrical aspect. Because of the spherical profile, the separation between two spheres will be a function of r, the distance from the centre of the contact area. The contact problem between two rough spheres is equivalent to the contact between a smooth sphere of radius R and a nominally rigid flat rough surface having a Gaussian distribution of asperities heights σ_s, where R and σ_s can be derived by the radii and roughness of the two spheres as

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \tag{1}$$

$$\sigma_s^2 = \sigma_{s1}^2 + \sigma_{s2}^2 \tag{2}$$

Then the contact pressure distribution is given by

$$p(r) = \frac{4}{3}E^* n\beta^{\frac{1}{2}} \int_{w(r)+\frac{r^2}{2R}}^{\infty} \left(z - \frac{r^2}{2R} - w(r)\right)^{3/2} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(z-\delta)^2}{2\sigma^2}} dz \tag{3}$$

where w(r) is the deformation of the sphere and can be obtained from the solution for the axi-symmetric deformation of an elastic half-space as follows

$$w(r) = \frac{4}{\pi E^*} \int_0^a \frac{t}{t+r} p(t)\boldsymbol{K}(k)dt \tag{4}$$

$$w(0) = \frac{2}{E^*} \int_0^a p(t)dt \tag{5}$$

in which $\boldsymbol{K}(k)$ is the first kind complete elliptic integral of $k = 2(rt)^{\frac{1}{2}}/(r+t)$, and a is the radius of the contact area for the smooth surfaces under the same load. Then the total contact force can be obtained by the integration of the pressure distribution over the contact area.

Clearly, the $p(r)$ distribution in the GW model involves a complicated integral with n, β and σ as the statistical characteristic parameters of surface roughness. In order to obtain $p(r)$, the nonlinear equations (3) and (4) have to be solved simultaneously, with the later also including a non-integrable part. A numerical method based on the Newton-Raphson iterations is applied to solve this problem. First, introduce $N+1$ discrete points along the contact radius. Then equation (3) must be satisfied at each point i:

$$p_i = \mu g(w_i) \tag{6}$$

where

$$\mu = \frac{4}{3}E^* n\beta^{\frac{1}{2}} \tag{7}$$

$$g(w_i) = \int_{w_i+\frac{r_i^2}{2R}}^{\infty} \left(z - \frac{{r_i}^2}{2R} - w_i\right)^{3/2} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(z-\delta)^2}{2\sigma^2}} dz \tag{8}$$

or in a different form

$$F_i(p_0, p_1, \dots, p_N) = p_i - \mu g(w_i) = 0 \tag{9}$$

which leads to a nonlinear system of equations for all the points:

$$\mathbf{F}(\mathrm{p}) = \mathrm{p} - \mu \mathrm{g} = 0 \tag{10}$$

To solve this system of equations in terms of p, function **F** is expanded by the Taylor series in neighbourhood of p as

$$\mathbf{F}(\mathrm{p} + \delta\mathrm{p}) = \mathbf{F}(\mathrm{p}) + \mathbf{J}\cdot\delta\mathrm{p} + \mathrm{O}(\delta\mathrm{p}^2) \tag{11}$$

where $\mathbf{J}$ is Jacobian matrix, which represents the gradient of the vector **F**. The value of $\mathbf{J}$ is obtained by a finite difference approximation. The increment $\delta\mathrm{p}$ is obtained by

$$\delta\mathrm{p} = -\mathbf{J}^{-1}\mathbf{F}(\mathrm{p}) \tag{12}$$

The solution p is achieved by the iterative process starting from a trial solution. Then the total contact force can be obtained by integrating the pressure $p(r)$ over the entire contact area. The $P{\sim}\delta$

relationships of two surfaces with different levels of roughness are shown in Fig. 1, in which the range of σ (normalised) is 0.0001~0.01 and δ (normalised) is 0~0.1. All the other parameters are set to be 1. The P~δ relationships of the Hertz law and the GW-model ($\sigma = 1.0e-4$) are shown in Fig. 2.

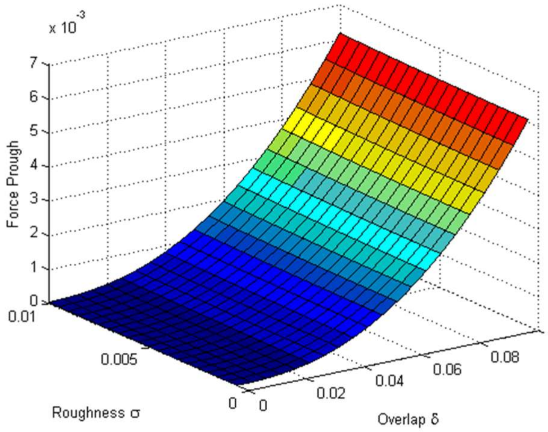

Figure 1: $P\sim\sigma\sim\delta$ relationships based on the numerical calculation

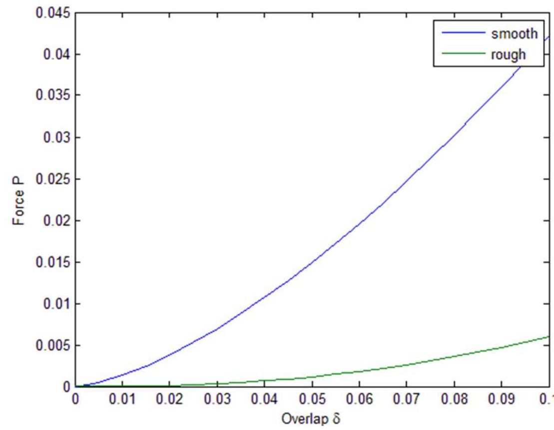

Figure 2: $P\sim\delta$ relationships of smooth surface and rough surface ($\sigma = 1.0e-4$)

3. Predictive formulas of the $P\sim\delta$ curve

In order to obtain the random normal interaction law that can be used in DEM, an explicit relationship between the total force P and the overlap δ needs to be defined from the numerical results via curve-fitting. It is of practical importance that the resulting relationship should have a simple closed form with the minimum number of added parameters. Equation (3) indicates that there are two added parameters, σ and $n\beta^{\frac{1}{2}}$, and that P is proportional to $n\beta^{\frac{1}{2}}$ (note that the numerical results obtained are for $n\beta^{\frac{1}{2}} = 1$).

It is obvious that the $P\sim\delta$ relationship should degenerate to the Hertz law when $\sigma = 0$. However, to treat $n\beta^{\frac{1}{2}}$ as an independent parameter from σ will violate this requirement as different values of $n\beta^{\frac{1}{2}}$ would lead to different $P\sim\delta$ curves at $\sigma = 0$. To resolve this issue, $n\beta^{\frac{1}{2}}$ is calibrated in the following way. When σ is sufficiently small, the rough surface should be regarded as a smooth surface and thus should have the same $P\sim\delta$ relationship as the Hertz law. However, Fig. 2 depicts a clear difference between P_{smo} and P_{rough} (with $n\beta^{\frac{1}{2}} = 1$, and assuming that $\sigma = 1.0e-4$ is sufficiently small). Our numerical calculation shows that the condition P_{rou} $(\sigma = 0) = P_{smooth}$ can be enforced if $n\beta^{\frac{1}{2}}$ takes the following value:

$$n\beta^{\frac{1}{2}} = \frac{P_{smooth}}{P_{rough}} = 0.62R^{-\frac{1}{2}}\delta^{-1} \tag{13}$$

Then σ now becomes the solely added parameter in the $P\sim\delta$ relationship, making the new interaction law much simpler. The correctness of this formula can be verified through the analysis of equation (3) at the special case $\sigma = 0$, based on the fact that the Gaussian distribution reduces to the Dirac Delta Function when $\sigma \to 0$:

$$\delta(t) = \lim_{\sigma\to 0} \frac{1}{\sqrt{2\pi}\sigma} e^{-t^2/2\sigma^2} \tag{14}$$

An important property of the delta function is that for a given function $f(x)$

$$\int f(t)\delta(t - t_0)dt = f(t_0) \tag{15}$$

Thus when $\sigma \to 0$, the pressure distribution $p(r)$ in equation (3) reduces to

$$p(r) = \frac{4}{3}E^* n\beta^{\frac{1}{2}}\left(\delta - \frac{r^2}{2R} - w(r)\right)^{3/2} \tag{16}$$

An explicit expression for $p(r)$ is not possible because of the inter-dependence between $p(r)$ and $w(r)$ which is the deformation of the smooth sphere. However, we artificially set $w(r) = 0$, which leads to an explicit but approximate expression for $p(r)$

$$p(r) = \frac{4}{3}E^*n\beta^{\frac{1}{2}}(\delta - \frac{r^2}{2R})^{3/2} \tag{17}$$

The total contact force can be obtained by the integration of the pressure distribution over the contact area as

$$P_{rough} = \int_0^a 2\pi r p(r)dr = 2.76E^*n\beta^{\frac{1}{2}}R\delta^{\frac{5}{2}} \tag{18}$$

The nominally flat rough surface can be considered as smooth surface when $\sigma \rightarrow 0$. The contact force between the sphere and the smooth surface can be calculated by the Hertz law

$$P_{smoot} \quad = \frac{4}{3}E^*R^{\frac{1}{2}}\delta^{\frac{3}{2}} \tag{19}$$

The condition P_{rough}= P_{smoot} gives rise to

$$n\beta^{\frac{1}{2}} = 0.48R^{-\frac{1}{2}}\delta^{-1} \tag{20}$$

which is the same as formula (13) except for a smaller coefficient. This discrepancy can be explained: the assumption $w(r)$=0 increases the overlap between the sphere and the asperities, thereby leading to a larger $p(r)$, and thus a larger P_{rough}, and therefore a smaller coefficient.

Based on the above analysis and applying curve-fitting, the predictive formula for calculating the normal contact force between two rough spheres is derived as (with the $Rsqure = 0.98$)

$$P_{rough} = E^*R^{\frac{1}{2}}\left(\frac{4}{3} - 39.13\sigma\right)\delta^{\left(\frac{3}{2}-9.57\ \right)} + 1.5\sigma^{2.5} \tag{21}$$

Cleary, when $\sigma = 0$, the formula recovers the Hertz law as required. Also, the total force is no longer zero when $\delta = 0$ for $\sigma > 0$ because some asperities of the two rough spheres may be in contact even there is no overlap between the two mean surfaces.

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