Formulation of Porosity Calculation for Three-Dimension Granular Materials in the Case of Spherical Particles

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Abstract. A derivation of formulation for calculating porosity of three-dimension granular materials is presented in this work, where granular particles are assumed spherical. Overlapping area problem is solved in two-dimension using geometry in two overlapping circles. The three-dimension overlap is formulated through numeric integration from the two dimension overlap.

Keywords: granular materials, porosity calculation, two-dimension overlap, spherical particles.

PACS: 45.70.Cc, 45.70.Mg, 81.05.Rm.

1 Introduction

Porosity calculation of two-dimension granular grains configurations produced from simulation can be performed using image processing [1]. Furthermore, this method can be advanced for three-dimensional structure by analyzing slice by slice results from X-ray micro-CT imaging [2, 3]. One of the reasons why structure information such as porosity is important, because it is related to bulk properties of the materials consisted of granular grains [4]. In this work, other method than image processing is proposed to calculate the porosity. The problem in overlapping spherical grains is also discussed.

2 Calculation of porosity

Considered that there are three-dimension grains configurations as illustrated in Figure 1, where from the simulation particle positions can be easily obtained, while from the experiment it is rather difficult. Assumed that particle positions and radius are already available

$$x_i, y_i, z_i, R_i, \quad i = 1,..,N. \tag{1}$$

On a horizontal plane z radius of spherical grains i will have circle equation

$$(x - x_i)^2 + (y - y_i)^2 = R_{i,z}^2, \tag{2}$$

where

$$R_{i,z}^2 = \max\left[0, R_i^2 - (z - z_i)^2\right]. \tag{3}$$

Projection of spherical grain i exists in plane z if $R_{i,z} > 0$. Requirement from Equation (3) will determine which grains should be included in calculating projection area of all grains in plane z.

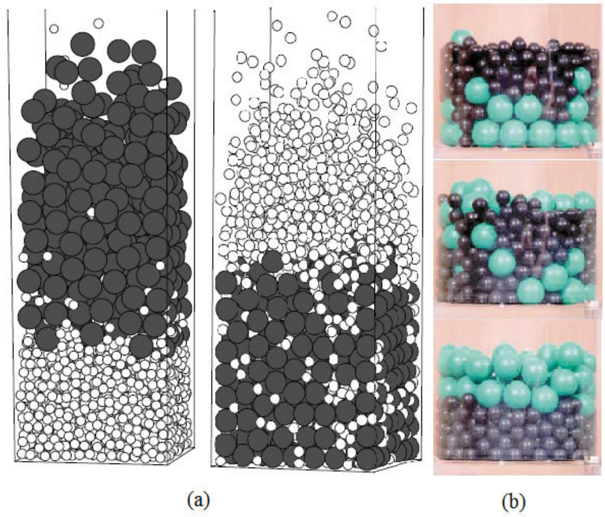

Figure 1. Example of three-dimension grains configuration as reported in: (a) simulation [5] and (b) experiment [6].

Non-overlapping grains

Porosity in a plane z can defined as

$$\phi_z = 1 - \frac{A_{g,z}}{A}. \tag{4}$$

where A is area of plane z and $A_{g,z}$ is area occupied by grains projection on the plane, which have circle equation from Equation (2). If the system is constrained in a box with dimension $p \times l \times h$ then

$$A = pl \,. \quad (5)$$

If there is no overlap between grains then $A_{g,z}$ will be simply as

$$A_{g,z} = \sum_{i=1}^{N} \pi R_{i,z}^2 \,. \quad (6)$$

For condition where there are overlaps, Equation (6) must be modified.

Overlapping grains

Figure 2 shows the difference between grains configurations where overlapping grains exists and where not. In the former case boundary of each grain projection can not be identified, while in the later case it still can.

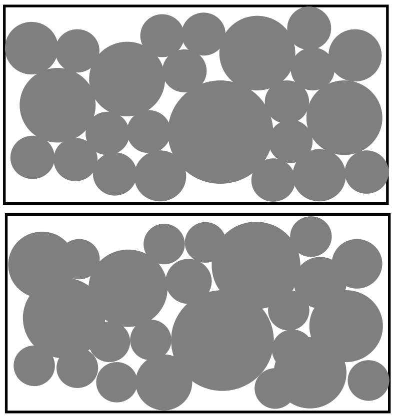

Figure 2. Grains projection on a plane z for condition: non-overlapping grains (top) and overlapping grains (bottom).

Considered first there are two grain projections in a plane z with radius R_i and R_j, whose centers are located at (x_i, y_i) and (x_j, y_j). Overlap between grains can be defined as [7]

$$\xi_{ij} = \max\left[0, R_i + R_j - r_{ij}\right] \,, \quad (7)$$

where

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \,. \quad (8)$$

Both Equations (3) and (7) uses function $\max()$, which is defined as

$$\max(x, y) = \begin{cases} x, & x \geq y, \\ y & x < y. \end{cases} \quad (9)$$

Meaning of overlap ξ_{ij} from Equation (7) is given in Figure 3 as illustration.

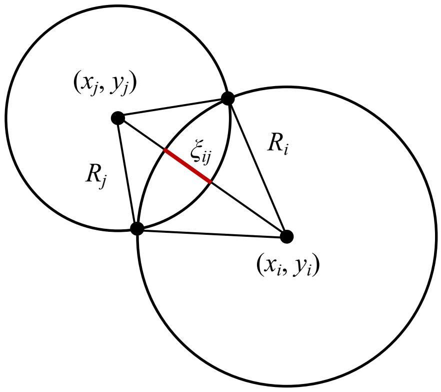

Figure 3. Overlap distance between two spherical grains grains i and j.

For clearer illustration area of interest from Figure 3 is redrawn in Figure 4. Sector of circle i with boundaries line R_i, circumference with angular distance θ_i, and line R_i has area of

$$A_{s,i} = \frac{1}{2} R_i^2 \theta_i \,, \quad (10)$$

and also for sector of circle j. Area of triangle in circle i with boundaries line R_i, chord l, and line R_i has area of

$$A_{t,i} = \frac{1}{2} R_i^2 \sin\theta_i \quad (11)$$

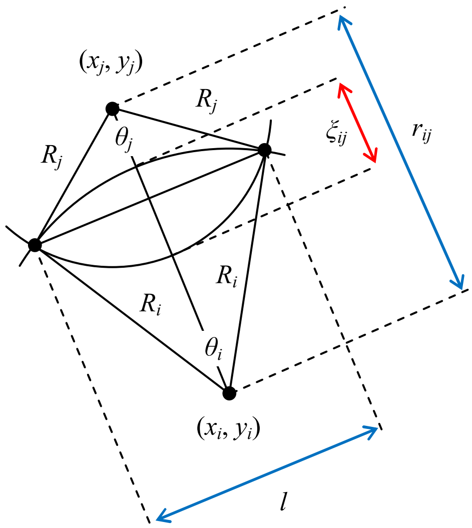

Figure 4. Overlap area between two grains i and j with other geometry parameters required for calculation the overlap area.

using half of vector cross product in calculating area of a parallelogram. Then, total area of circle i minus the overlap segment is

$$A_{o,i} = A_{c,i} - A_{s,i} + A_{t,i} \,, \quad (12)$$

where $A_{c,i}$ is circle are

$$A_{c,i} = \frac{1}{2} R_i^2 2\pi \ . \tag{13}$$

Substitution of Equations (10), (11), and (13) into Equation (12) will produce

$$A_{o,i} = \frac{1}{2} R_i^2 \left(2\pi - R_i^2 \theta_i + \sin\theta_i\right). \tag{14}$$

Then, total area occupied by projection of spherical grains *i* and *j* in plane *z* is

$$A_{z,ij} = \frac{1}{2}\left[R_i^2 \left(2\pi - \theta_i + \sin\theta_i\right) \right. \\ \left. R_j^2 \left(2\pi - \theta_j + \sin\theta_j\right)\right] \tag{15}$$

Equation (6) can be modified using Equation (15) into

$$A_{g,z} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} A_{z,ij} \ . \tag{16}$$

Equation (15) will reduce to Equation (6) if $\theta_i = \theta_j = 0$ or there is no overlapping grains in plane z. Equation (15) still requires value of θ_i and θ_j, where the way how to find them will be shown in next subsection.

Angle of overlapping area

From Figure 4 following relation can be obtained

$$\begin{aligned} &\left(\frac{l}{2}\right)^2 = R_j^2 - h_j^2 = R_i^2 - h_i^2 \\ &\Rightarrow h_i^2 - h_j^2 = R_i^2 - R_j^2 \\ &\Rightarrow \left(h_i - h_j\right)\left(h_i + h_j\right) = R_i^2 - R_j^2 \\ &\Rightarrow \left(h_i - h_j\right) r_{ij} = R_i^2 - R_j^2 \\ &\Rightarrow h_i = h_j + \frac{R_i^2 - R_j^2}{r_{ij}} \\ &\Rightarrow h_i = \left(r_{ij} - h_i\right) + \frac{R_i^2 - R_j^2}{r_{ij}} \\ &\Rightarrow h_i = \frac{1}{2} r_{ij} + \frac{R_i^2 - R_j^2}{2 r_{ij}} \end{aligned} \tag{17}$$

and also

$$\begin{aligned} &\frac{h_i}{R_i} = \cos\frac{\theta_i}{2} \\ &\Rightarrow \cos\theta_i = 2\left(\frac{h_i}{R_i}\right)^2 - 1 \\ &\Rightarrow \sin\theta_i = \sqrt{1 - \left[2\left(\frac{h_i}{R_i}\right)^2 - 1\right]^2} \ . \end{aligned} \tag{18}$$

Similar relations for θ_j can be shown for Equations (17) and (18) straight forwards.

Total porosity

A system constrained in a box with dimension $p \times l \times h$ at plane z it will has area occupied by overlapping grains

$$A_{g,z} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \frac{1}{2}\left[R_{i,z}^2 \left(2\pi - \theta_i + \sin\theta_i\right) \right. \\ \left. R_{j,z}^2 \left(2\pi - \theta_j + \sin\theta_j\right)\right] \tag{19}$$

which implicitly depends on z. Sum over z will produce total volume occupied by all overlapping spherical grains

$$V_g = \int_0^h A_{g,z} dz = \sum_{k=1}^{M} A_{g,z} \, \Delta z \ , \tag{20}$$

with

$$z = (k-1)\Delta z \tag{21}$$

and

$$\Delta z = \frac{h}{M-1} \ . \tag{22}$$

Then, total porosity of the system will be

$$\phi = 1 - \frac{V_g}{V} \ , \tag{23}$$

where

$$V = plh \ . \tag{24}$$

3 Summaries

Derivation of formula for porosity calculation for three-dimension granular materials has been presented in this work. Further investigation is required to justify result.

Acknowledgements

This work is supported financially by Hibah Desentralisasi DIKTI under scheme of Penelitian Unggulan Perguruan Tinggi in year 2015.

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