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Numerical simulation of tetrahedral particle mixing and motion in rotating drums

Nan Gui[a], Xingtuan Yang[a], Jiyuan Tu[a,b], Shengyao Jiang[a,*], Zhen Zhang[a]

[a] Institute of Nuclear and New Energy Technology, Collaborative Innovation Center of Advanced Nuclear Energy Technology, Key Laboratory of Advanced Reactor Engineering and Safety of Ministry of Education, Tsinghua University, Beijing 100084, China
[b] School of Engineering, RMIT University, Melbourne, VIC 3083, Australia

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ABSTRACT

A regular tetrahedron is the simplest three-dimensional structure and has the largest non-sphericity. Mixing of tetrahedral particles in a thin drum mixer was studied by the soft-sphere-imbedded pseudo-hard particle model and compared with that of spherical particles. The two particle types were simulated with different rotation speeds and drum filling levels. The Lacey mixing index and Shannon information entropy were used to explore the effects of sphericity on the mixing and motion of particles. Moreover, the probability density functions and mean values and variances of motion velocities, including translational and rotational, were computed to quantify the differences between the motion features of tetrahedra and spheres. We found that the flow regime depended on the particle shape in addition to the rotation speed and filling level of the drum. The mixing of tetrahedral particles was better than that of spherical particles in the rolling and cascading regimes at a high filling level, whereas it may be poorer when the filling level was low. The Shannon information entropy is better than the Lacey mixing index to evaluate mixing because it can reflect the real change of flow regime from the cataracting to the centrifugal regime, whereas the mixing index cannot.

Introduction

Particulate materials and their assemblies are far from well understood because they have rather complicated properties and flow behavior. Size and shape are the two most commonly used parameters to describe particles (Taylor, 2002). The scales of particles in different industries may range from nanometer to large gravels (Zhang, Lu, Wang, & Li, 2008). Meanwhile, shape also influences the microscopic behavior and macroscopic properties of granular media, e.g., polarizability and viscosity (Bullard & Garboczi, 2013). However, vast amounts of data are usually needed to characterize particle shape. Various shape descriptors have been used in the modeling of particle flows (Abou-Chakra, Baxter, & Tüzün, 2004).

Because of their easy and accurate description, modeling, and measurement, particles with regular shapes, e.g., circle/sphere, square/cube, and triangle/tetrahedron, are of fundamental importance in research related to drag (Hölzer & Sommerfeld, 2009; Loth, 2008; Wachs, 2009; Yow, Pitt, & Salman, 2005), mixing (Liu et al., 2017; Nafsun et al., 2017), and packing (Boon, Houlsby, & Utili, 2013; Wachs, Girolami, Vinay, & Ferrer, 2012). In particular, shape must be considered in particle packing, because the packing of non-spherical particles is considerably different from that of spherical particles (Li, Zhao, Lu, & Xie, 2010). The tetrahedron is a fundamental shape with many important features. For example, for common objects, the sphericity is the largest for a sphere (1) and the lowest for a regular tetrahedron (0.671) (Li, Li, Zhao, Lu, & Meng, 2012). In other words, a regular tetrahedron can be regarded as the most non-spherical shape, which means it has the lowest flowability. Modeling a polyhedron using the discrete element method (DEM) is much more complex than the modeling of many other non-spherical shapes like spherocylinders (Meng & Li, 2017) and ellipsoids (Zhao, Zhou, Liu, & Lai, 2015). They also mentioned that the study of tetrahedral materials is important in geotechnical, mining, and transportation engineering.

DEM-based methods are the most attractive techniques for modeling non-spherical particle shapes (Lu, Third, & Muller, 2015; Wachs et al., 2012). Wachs et al. (2012) used a variant of DEM named Grains3d to cope with convex non-spherical particles by

* Corresponding author.
E-mail addresses: guinan@mail.tsinghua.edu.cn, zjuguinan@zju.edu.cn (N. Gui), shengyaojiang@sina.com (S. Jiang).

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Nomenclature

D	Drum diameter
$f(\cdot)$	Function
$\boldsymbol{f}_{i,\mathrm{ms}}$	Contact force vector of member sphere i
$\boldsymbol{g}$	Gravity acceleration
$\boldsymbol{G}$	Gravity force of tetrahedron
$\boldsymbol{I}_{\mathrm{tet}}$	Moment of inertia of tetrahedron
k_{c}	Stiffness factor for particle collision
k_{r}	Stiffness factor of the restoring force in the relaxation process
m_{s}	Mass of member sphere
M_{tet}	Mass of tetrahedron
M_{I}	Mixing index
M_{E}	Shannon information entropy
n_{A}, n_{B}	Concentrations of two predefined types of particles
$\boldsymbol{n}_{i,\mathrm{ms}}$	Unit vector in the normal direction in collision for member sphere i
N_{p}	Number of tetrahedrons
N_{s}	Number of member spheres in *a* tetrahedron
N_{ϕ}	Number of data points for ϕ
P	Overall proportion of particle
$\boldsymbol{r}_{i,\mathrm{ms}}$	Position vector of member sphere i with respect to tetrahedron centroid
$\boldsymbol{R}_{i,\mathrm{ms}}$	Restoring force of member sphere i pointing to the equilibrium position
s, s_0, s_r	Standard deviations at unmixed state and randomly mixed state
t	Time
$\boldsymbol{t}_{i,\mathrm{ms}}$	Unit vector in the tangential direction in collision for member sphere i
$\boldsymbol{T}_{i,\mathrm{ms}}$	Torque of the tetrahedral particle caused by the member sphere i
u_{p}	Magnitude of particle velocity components
v_i	Velocity vector of member sphere i
$\boldsymbol{V}_{j,\mathrm{tet}}$	Velocity vector of tetrahedron j
$\boldsymbol{V}_{\mathrm{p}}$	Particle velocity vector
$\delta\boldsymbol{x}_{i,\mathrm{ms}}$	Displacement vector of member sphere i in collision
$\boldsymbol{\delta\xi}_{i,\mathrm{ms}}$	Displacement vector of member sphere i in the relaxation process
ΔT	Interval
$\boldsymbol{\Theta}_{j,\mathrm{tet}}$	Rotational velocity vector of tetrahedron
η_{c}	Damping coefficient in collision
η_{r}	Damping coefficient in the relaxation process
σ	Variance
ω	Rotating velocity of drum
μ	Coefficient of friction

Subscripts

c	Collision or contact
i, j	Indices
ms	Member sphere
p	Particle
r	Restoring
tet	Tetrahedron
x, y	Directions of coordinates

using the Gilbert–Johnson–Keerthi algorithm to compute the distance between convex bodies. They demonstrated the capability of their method to model regular shapes including a sphere, cylinder, cube, and tetrahedron. However, they did not compare tetrahedra and spheres to a sufficient extent to provide details of the effects of particle shape on mixing in a drum. Recently, out group proposed the soft-sphere-imbedded pseudo-hard particle model (SIPHPM), which has been validated for modeling of non-spherical shapes (Gui, Yang, Jiang, & Tu, 2016). In this work, we use the SIPHPM method to simulate the motion and mixing of tetrahedral particles in a drum mixer. The main purpose of this work is to compare the mixing and motion of regular tetrahedra with those of spheres to determine the effects of shape on particle mixing and motion in drums.

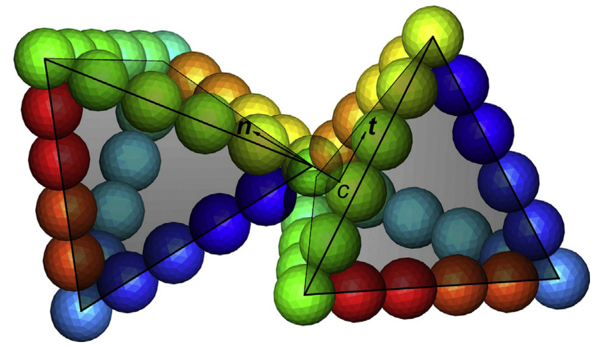

Fig. 1. Sketch of a surface collision between member spheres of two tetrahedral particles.

Methodology

SIPHPM

The SIPHPM (Gui et al., 2016) was used here to simulate the collision between tetrahedral particles. The particles were all uniform regular tetrahedra. Each was composed of 28 member spheres enclosing six surfaces (Fig. 1). Each tetrahedron was assumed to be composed of a pseudo-rigid material that was always undeformable. The collision between tetrahedra was solved through the collision between the member spheres and surfaces enclosed by the member spheres. In addition, the member spheres could deviate slightly from their equilibrium positions. A restoring force was always generated once a deviation occurred. The equilibrium positions of member spheres were on the vertexes and sides of each tetrahedron and determined by the position and orientation of the tetrahedron. The governing equations of the tetrahedra and member spheres were coupled and solved as follows:

For the member spheres:

$$\begin{cases} \boldsymbol{f}_{i,\mathrm{ms}} = k_{\mathrm{c}}\boldsymbol{\delta x}_{i,\mathrm{ms}} - \eta_{\mathrm{c}}\boldsymbol{\delta\dot{x}}_{i,\mathrm{ms}}, \\ \text{if}\langle \boldsymbol{f}_{i,\mathrm{ms}}, \boldsymbol{t}_{i,\mathrm{ms}}\rangle > \mu\langle \boldsymbol{f}_{i,\mathrm{ms}}, \boldsymbol{n}_{i,\mathrm{ms}}\rangle, \text{then}\langle \boldsymbol{f}_{i,\mathrm{ms}}, \boldsymbol{t}_{i,\mathrm{ms}}\rangle = \mu\langle \boldsymbol{f}_{i,\mathrm{ms}}, \boldsymbol{n}_{i,\mathrm{ms}}\rangle \\ \boldsymbol{T}_{i,\mathrm{ms}} = \boldsymbol{r}_{i,\mathrm{ms}} \times \boldsymbol{f}_{i,\mathrm{ms}}, \\ \boldsymbol{R}_{i,\mathrm{ms}} = k_{\mathrm{r}}\boldsymbol{\delta\xi}_{i,\mathrm{ms}} - \eta_{\mathrm{r}}\boldsymbol{\delta\dot{\xi}}_{i,\mathrm{ms}}, \\ \dot{\boldsymbol{v}}_i = \left(\boldsymbol{f}_{i,\mathrm{ms}} + \boldsymbol{R}_{i,\mathrm{ms}}\right)/m_{\mathrm{s}} - \boldsymbol{g}, \end{cases} \tag{1}$$

where $\delta\boldsymbol{x}_{i,\mathrm{ms}}$, $\boldsymbol{r}_{i,\mathrm{ms}}$, and $\boldsymbol{\delta\xi}_{i,\mathrm{ms}}$ are the deformation displacement, position vector (relative to the center of the tetrahedron), and deviation displacement from the equilibrium position of the ith member sphere, respectively; $\boldsymbol{f}_{i,\mathrm{ms}}$, $\boldsymbol{R}_{i,\mathrm{ms}}$, and $\boldsymbol{T}_{i,\mathrm{ms}}$ are the damping elastic collision force, restoring force, and torque of the ith member sphere, respectively; $\boldsymbol{n}$ and $\boldsymbol{t}$ are the normal and tangential directions at the collision point, respectively; $\boldsymbol{g}$ is the gravity acceleration; k_{c}, k_{r}, η_{c}, and η_{r} are the stiffness factors (k_x) and damping coefficients (η_x) of collision (denoted by subscript 'c') and restoration (denoted by subscript 'r'), respectively; μ is the friction coefficient for member spheres; v_i and m_{s} are the velocity and mass of the member spheres, respectively; and '$\langle\cdot\rangle$' is the inner operator.