Powder Technology 311 (2017) 157–166

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Effect of particle shape and size on effective thermal conductivity of packed beds

Jieqing Gan, Zongyan Zhou *, Aibing Yu

Laboratory for Simulation and Modelling of Particulate Systems, Department of Chemical Engineering, Monash University, Clayton, VIC 3800, Australia

ARTICLE INFO

Article history:
Received 17 March 2016
Received in revised form 5 November 2016
Accepted 6 January 2017
Available online 31 January 2017

Keywords:
Discrete element method
Effective thermal conductivity
Ellipsoids
Heat transfer
Packed beds

ABSTRACT

Effective thermal conductivity (ETC) is one of the most important thermal properties of packed granular materials, and is affected significantly by particle properties. In this work, discrete element method is used to study the effect of particle shape and size on the ETC of packed beds with ellipsoidal particles. The simulated ETC results are verified by experimental data with a good agreement. It is revealed that for coarse particles, the bed ETC increases with aspect ratio of ellipsoids deviating from 1.0. But for fine particles, the effect of aspect ratio becomes less significant. Such an effect is closely related to the difference of packing structures of ellipsoids at different sizes and aspect ratios. The results also reveal that at low particle thermal conductivity, the ETC is not affected much by particle size; at high particle thermal conductivity, the ETC increases with particle size. When bed temperature increases, the ETC increases markedly. The contributions of different heat conduction paths under different conditions are also quantified.

1. Introduction

Effective thermal conductivity (ETC) is a commonly used parameter to describe the overall thermal performance of packed beds. Packing structure, which is usually affected by particle size and shape, packing method, external mechanical load, mechanical and surface properties of solid particles [1,2], can significantly affect the bed ETC. In the past decades, extensive experimental ETC data have been generated and analyzed in the literature [3–6]. However, the underlying heat transfer mechanisms in packed beds are usually difficult to be quantified by physical experiments. Alternatively, mathematical modelling offers an effective way to investigate the heat transfer fundamentals in fluid bed reactors. Various mathematical models including continuum models and microscopic models have been proposed, but they are often limited by the homogeneity assumptions in continuum models [7–10] or simple assumptions in microscopic models [11–13]. In recent years, the combined approach of discrete element method (DEM) and computational fluid dynamics (CFD) has been successfully applied in the study of heat transfer in packed and fluidized beds [14–16], taking into account most of the known heat transfer mechanisms, including particle-fluid/fluid-wall convection, particle-particle/particle-wall conduction, and particle radiation [17–21].

However, the idealized spherical shape of particles is usually used in the DEM simulation. In practice, most of particle shapes differ substantially from spheres. Generally speaking, particle shape can affect packing structures that are critical to transport properties such as permeability related to pore connection and thermal conductivity related to particle connection. For example, ellipsoids can pack more densely than spheres [21], and the dependence of bed porosity on particle shape can be observed for coarse cylinders and disks [22]. Hence, particle shape can affect the bed thermal performance significantly. For example, the experimental data [10] showed that bed ETC increases with decreasing particle sphericity. The similar tendency was also found in the dilute system of nanoparticle suspensions [23]. A sphericity term has been introduced to theoretical models [10,24] to account for the effect of particle shape. However, up to date, the experimental ETC data for nonspherical particles is still very limited [10,6], and the effect of particle shape have not been fully quantified.

In our recent work, the heat transfer models used for spheres have been extended to ellipsoids in packed and fluidized beds [16]. In this work, the analytical solutions to the problem of conductive heat transfer for oblate and prolate ellipsoids are introduced first. Then we focus on studying the effects of aspect ratio of ellipsoids, particle thermal conductivity, and particle size on the ETC of packed beds. The heat transfer mechanisms in terms of contributions of different heat transfer modes are also quantified.

2. Simulation method

2.1. Governing equations

DEM, as a dynamic mathematical model, has been widely used to study particle packing under various conditions, including packings of

* Corresponding author.
E-mail address: zongyan.zhou@monash.edu (Z. Zhou).

http://dx.doi.org/10.1016/j.powtec.2017.01.024

Table 1
Components of forces and torque acting on particle *i*.

Forces and torques	Symbols	Equations
Normal elastic force	$\mathbf{f}_{cn,ij}$	$-{}^4/{}_3 E^* \sqrt{R^*} \delta_n^{3/2} \mathbf{n}$
Normal damping force	$\mathbf{f}_{dn,ij}$	$-c_n (8 m_{ij} E^* \sqrt{R^* \delta_n})^{1/2} \mathbf{v}_{n,ij}$
Tangential elastic force	$\mathbf{f}_{ct,ij}$	$-\mu_s \lvert \mathbf{f}_{cn,ij} \rvert (1-(1-\delta_t/\delta_{t,\max})^{3/2}) \hat{\boldsymbol{\delta}}_t \quad (\delta_t < \delta_{t,\max})$
Tangential damping force	$\mathbf{f}_{dt,ij}$	$-c_t (6 \mu_s m_{ij} \lvert \mathbf{f}_{cn,ij} \rvert \sqrt{1-\lvert V_t \rvert/\delta_{t,\max}} / \delta_{t,\max})^{1/2} \mathbf{v}_{t,ij}$ $(\delta_t < \delta_{t,\max})$
Coulomb friction force	$\mathbf{f}_{t,ij}$	$-\mu_s \lvert \mathbf{f}_{cn,ij} \rvert \hat{\boldsymbol{\delta}}_t \quad (\delta_t \geq \delta_{t,\max})$
Torque by normal force	$\mathbf{M}_{n,ij}$	$\mathbf{R}_{ij} \times (\mathbf{f}_{cn,ij} + \mathbf{f}_{dn,ij})$
Torque by tangential force	$\mathbf{M}_{t,ij}$	$\mathbf{R}_{ij} \times (\mathbf{f}_{ct,ij} + \mathbf{f}_{dt,ij})$
Rolling friction torque	$\mathbf{M}_{r,ij}$	$\mu_{r,ij} \lvert \mathbf{f}_{n,ij} \rvert \hat{\boldsymbol{\omega}}_{t,ij}^n$
Van der Waals force	$\mathbf{f}_{vdw,ij}$	$-A_{ij} \eta_{ij} \chi_{ij} \sigma [a/(a+0.5h_{ij})]^4 [c/(c+0.5h_{ij})]^2 / (12 h_{ij}{}^2)$

where, $1/m_{ij} = 1/m_i + 1/m_j$, $1/R^* = 1/\lvert R_i \rvert + 1/\lvert R_j \rvert$, $E^* = E/2(1-v^2)$, unit vector $\hat{\boldsymbol{\omega}}_{t,ij} = \boldsymbol{\omega}_{t,ij}/\lvert \boldsymbol{\omega}_{t,ij} \rvert$, $\delta_n = \lvert \boldsymbol{\delta}_n \rvert$, $\delta_t = \lvert \boldsymbol{\delta}_t \rvert$, unit vector $\hat{\boldsymbol{\delta}}_t = \boldsymbol{\delta}_t / \lvert \boldsymbol{\delta}_t \rvert$, $\delta_{t,\max} = \mu_s (2-v)/2(1-v) \cdot \delta_n$, $\mathbf{v}_{ij} = \mathbf{v}_j - \mathbf{v}_i + \boldsymbol{\omega}_j \times$-$_{ij} = \mathbf{v}_j - \mathbf{v}_i + \boldsymbol{\omega}_j \times \mathbf{R}_j - \boldsymbol{\omega}_i \times \mathbf{R}_i$, $\mathbf{v}_{n,ij} = (\mathbf{v}_{ij} \cdot \mathbf{n}) \cdot \mathbf{n}$, $\mathbf{v}_{t,ij} = (\mathbf{v}_{t,ij} \times \mathbf{n}) \times \mathbf{n}$, *a*, *b*, and *c* are the three principal semi-axis of the ellipsoid *i*; h_{ij} is the minimum surface separation, A_{ij} is the Hamaker constant, $\eta_{ij}\chi_{ij}$ is a coefficient dependent both on the orientation and relative position, and σ is the atomic/particle interaction radius. More details for the derivation of $\mathbf{f}_{vdw}$ for ellipsoids are given elsewhere [41]. Note that tangential forces ($\mathbf{f}_{ct,ij} + \mathbf{f}_{dt,ij}$) should be replaced by $\mathbf{f}_{t,ij}$ when $\delta_t > \delta_{t,\max}$.

ellipsoids [25–29]. When coupled with fluid flow, CFD-DEM approach for ellipsoids has also been developed [30,31]. In this work, the effect of fluid flow on the ETC is not considered, hence only DEM is used. A brief description of the DEM method for ellipsoids is given below.

According to the DEM, a particle can have two types of motion: translational and rotational, which are determined by Newton's second law of motion. The governing equations for the translational and rotational motion, and energy balance of particle *i* with mass m_i, moment of inertia I_i, and specific heat $c_{p,i}$ can be written as

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{k_c} \left(\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij} \right) + m_i \mathbf{g} + \mathbf{f}_{vdw} \tag{1}$$

$$\mathbf{I}_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{k_c} \left(\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij} + \mathbf{M}_{n,ij} \right) \tag{2}$$

$$m_i c_{p,i} \frac{dT_i}{dt} = \sum_{j=1}^{k_i} Q_{i,j} + Q_{i,rad} \tag{3}$$

where $\mathbf{v}_i$ and $\boldsymbol{\omega}_i$ are the translational and angular velocities of the particle *i*, respectively. T_i is the particle temperature. The forces involved are: the gravitational force $m_i\mathbf{g}$, and inter-particle forces between particles which include elastic force $\mathbf{f}_{c,ij}$ and viscous damping force $\mathbf{f}_{d,ij}$. For fine particles, the van der Waals force $\mathbf{f}_{vdw}$ should be considered. The torques include: $\mathbf{M}_{t,ij}$ by the tangential force, $\mathbf{M}_{r,ij}$ by the rolling friction, and $\mathbf{M}_{n,ij}$ generated by the normal force when the normal force does not pass through the particle centre. Equations used to calculate the interaction forces and torques between two spheres have been well-established [32] and extended to ellipsoids [30,21]. For convenience, they are given in Table 1. $Q_{i,j}$ is the heat transfer rate between particles *i* and *j* due to conduction, $Q_{i,rad}$ is the heat transfer rate between particle *i* and its surrounding environment by radiation. Note that in the present work, the heat transfer between particles and wall is not considered.

2.2. Heat transfer models

In this work, we focus on the heat transfer in packed beds with stagnant fluid where only conductive and radiative heat transfer occurs. Fig. 1 shows the heat conduction between two neighboring ellipsoids. In the literature, for smooth-elastic spheres, Vargas and McCarthy [33] considered the effect of stagnant interstitial fluids, and calculated the total thermal conduction by summing the contributions of three mechanisms including: (i) through the area of contact between particles, (ii) through the gas phase, and (iii) through the liquid phase. Similar treatments have also been done for spheres by other authors [14,15]. For example, conductive heat transfer between two spherical particles includes two heat transfer paths [33,14,15]: particle-fluid-particle heat transfer path and particle-particle heat transfer path. More details for the calculation of the two heat transfer modes can be found in our previous paper [16]. For convenience, they are briefly described below.

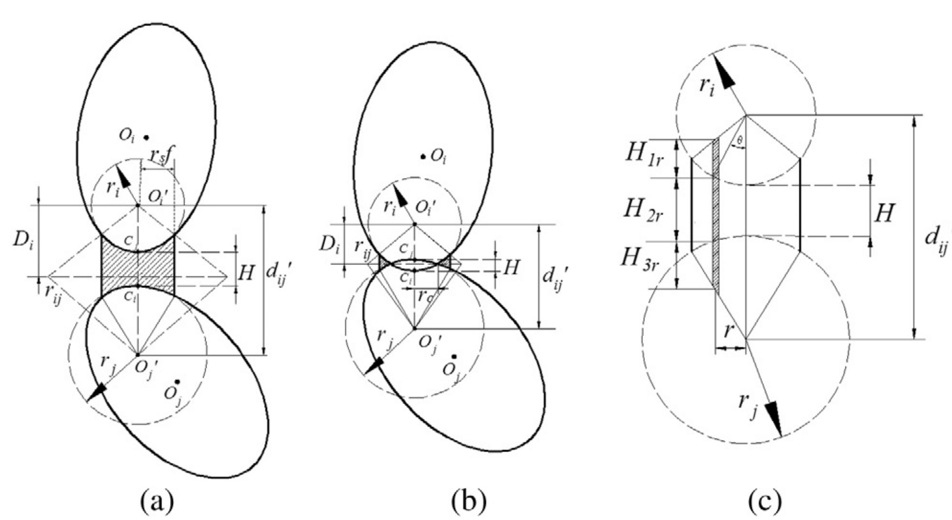

Fig. 1. Heat conduction model between two neighboring ellipsoids: (a) non-contact, (b) contact with an overlap, and (c) integral region in (a).