Correlation of Conductive Flux and Contact Stress – Lessons Learned from Simple Shear

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Abstract

Granular materials are used in numerous industrial processes such as mixing, drying, combustion, CO_2 and SO_2 capture, or hopper flows. In this paper we perform Discrete Element Method (DEM)-based simulations of heat conduction in a simple shear flow. The goal is to find a correlation between the heat flux and the particle-phase stress in various flow regimes. Such a correlation is of major importance, e.g., for reactive fluidized bed simulations where a closure for the effective heat conductivity of the particle-phase is needed.

Introduction

Granular materials show extremely complex flow features, and the development of simple models to describe the behavior of granular materials is still an ongoing task. While for the rheology good models are available (see, e.g., Chialvo et al [1]), there is only a basic understanding of the transport of thermal energy [2,3]. In this study, the conductive flux q^{cond} [W/m^2] and the contact stress for dilute and dense flow regimes are measured from simulations. This is a first step towards a more rigorous continuum-based model for (heat) conduction in a granular material. Such a model is of paramount industrial importance, e.g., to estimate the local temperature of particles more reliably in fluidized bed combustion, mixing, drying or coating applications.

Simulation Method and setup

Computer simulations were performed using the package LIGGGHTS [4]. A Linear-spring dashpot (LSD) model based on Hooke's theory has been used in this study [5], and the heat flux due to a single particle-particle collision has been modelled using the following equation:

$$Q_{tot} = K \cdot C \cdot T_{ref} \cdot \delta_c \cdot D \cdot (\theta_i - \theta_j). \tag{1}$$

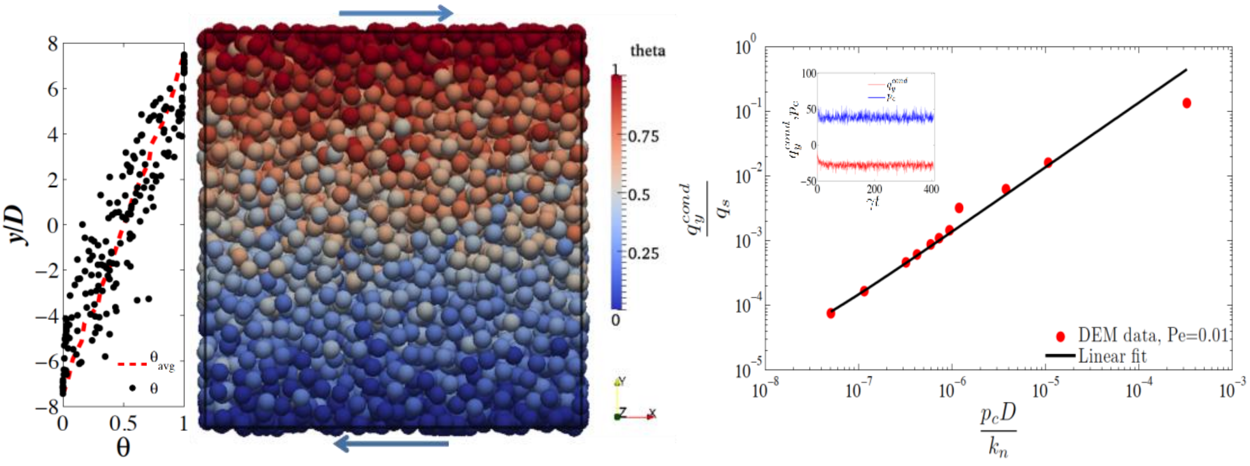
Here δ_c is the contact overlap, D is the diameter of the particles [m], C is a stiffness constant [1], T_{ref} is a reference temperature difference [K], θ is the dimensionless temperature of the particle, Q_{tot} is the rate of heat exchanged [W], and K is the thermal conductivity of the particle's material [W/mK].
Besides the particle volume fraction ϕ_p, the Peclet number

$$Pe = \frac{(D/2)^2}{K/\rho_p c_p} \cdot \gamma \tag{2}$$

can be identified as the main non-dimensional influence parameter (γ is the shear rate [$1/s$], ρ_p is the particle density, and c_p is the thermal capacity [$J/kg.K$]). In typical applications, this Peclet number ranges from 10^{-5} to 10^3. Here we focus only on $Pe = 0.01$.

Results

By performing shear flow simulations using Lees-Edwards boundary conditions [6], we are able to calculate the particle-phase stress and the heat fluxes *q* [W/m²] (conductive and convective) from particle information. We make the particles appropriately stiff to model granular materials (i.e., we choose $\gamma^* = 10^{-3}$, [1]). Particles were placed in a cubic periodic box (size $H = 15 \cdot D$), where particles near the top boundary were fixed to be hot ($\theta_1=1$) and near the bottom boundary were fixed to be cold ($\theta_0=0$). We can now define $q_s = -K \nabla_y T$ as the reference conductive heat flux ($\nabla_y T$ being the imposed temperature gradient). As the particles are sheared in the *x*- (i.e., streamwise) direction, the particles collide with each other and exchange heat. This imposes a linear (mean) temperature profile on the shear flow (see Fig 1a), while individual particles' temperature scatter around this mean profile (see Fig 1b). The latter is a result of granular diffusion, i.e., the random motion of particles. Fig 1(c) shows our first results for the correlation of the contact pressure and the conductive heat flux. Based on this correlation, one could now attempt to model the heat flux based on a rheological model (e.g., the particle-phase pressure model of Chialvo et al. [1]).



(a) (b) (c)

Figure 1: (a) Temperature profile of particles along the gradient (i.e., y) direction, (b) snapshot of the particle temperature distribution for $\phi_p = 0.3$, (c) scaled conductive heat flux in the gradient direction vs. the scaled contact pressure (red dots indicate results for different particle volume fractions; the insert shows the temporal fluctuations of the pressure and the conductive heat flux for $\phi_p = 0.59$).

Conclusion

We demonstrated the use of LIGGGHTS for a detailed analysis of stress and (thermal) heat flux in shear granular materials. Our results point to an interesting finding, namely that there exists a connection between stress properties (i.e., the contact stress) and the conductive transport within a particle bed. Using this connection might be useful to model the transport of thermal energy, and other scalar quantities (e.g., the amount of liquid on particles) within a bed of moving particles.

Acknowlegement

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