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A Model for the Conductive Heat Flux in Granular Flows based on a Correlation with the Contact Pressure

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(Project P23627)

Introduction

Granular materials show extremely complex flow features, and the development of simple models to describe the behavior of these materials is still an on-going 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 in flowing granular materials [2,3]. For example, Rognon et al. [2] could establish a model for the conductive heat flux only in a single flow regime. A more rigorous model (valid for all flow regimes) would be of paramount industrial importance, e.g., to predict the local temperature of particles more reliably in fluidized bed combustion, mixing, drying or coating applications.

Here we build a model for the conductive heat flux q^{cond} [W/m^2] by correlating q^{cond} to the contact pressure p_c [N/m^2]. Specifically, we have measured both quantities from discrete element method (DEM) based simulations.

Simulation Method and Setup

Computer simulations were performed using the package LIGGGHTS [4]. A linear-spring dashpot (LSD) model has been used in this study [5], and the heat exchange rate Q_{tot} in a single particle-particle collision has been modeled using the following equation:

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

K thermal conductivity $[W/mK]$	δ_c dimensionless contact overlap $[-]$
T_{ref} reference temperature difference $[K]$	D diameter of the particle $[m]$
γ shear rate $[1/s]$	C stiffness constant
θ dimensionless temperature of the particle $[-]$	Q_{tot} rate of heat exchanged $[W]$
ρ_p particle density $[kg/m^3]$	c_p heat capacity $[J/kg \cdot K]$

Besides the particle volume fraction ϕ_p, the Peclet number

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

can be identified as the main non-dimensional influence parameter. The coefficient of normal restitution e_n and the coefficient of friction μ are chosen as 0.9 and 0.10. In typical applications, this Peclet number ranges from 10^{-5} to 10^{3}. Here, we focus only on *Pe* = 0.01, 1.0 and 100.

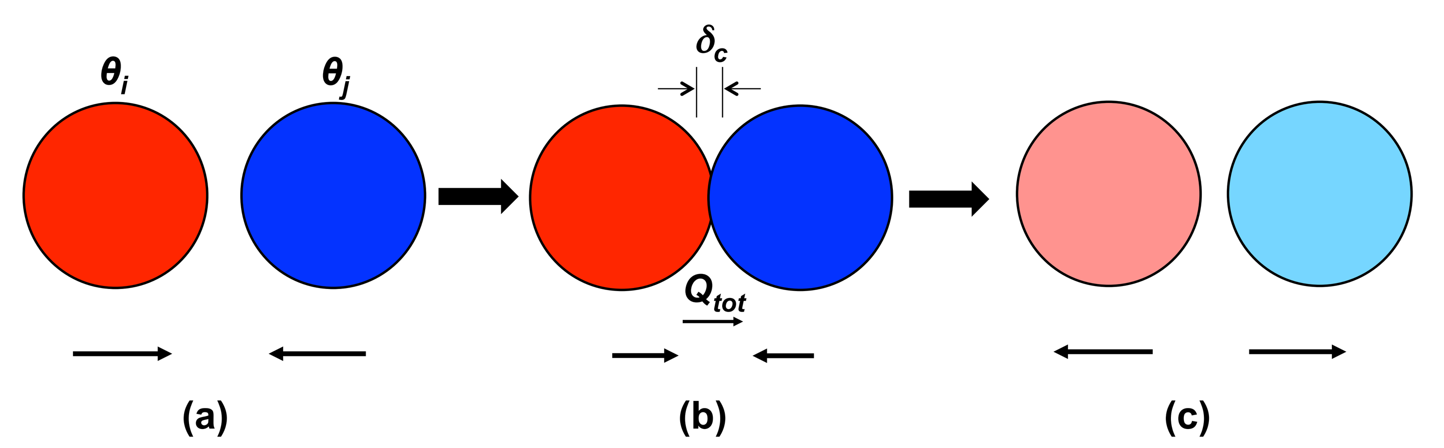

Fig. 1: Schematic representation of the heat conduction between two particles: (a) hot and cold particles approach each other, (b) particles collide and heat transfer takes place, (c) particles bounce away from each other.

We make the particles appropriately stiff to model granular materials (i.e., we choose the dimensionless shear rate ($\gamma* = \gamma D/\sqrt{k_n/\rho_p D}$) to be 10^{-3}, [1], where k_n is spring stiffness). Particles were placed in a cubic periodic box (size $H = 15 \cdot D$). Particles near the top boundary were fixed to be hot ($\theta_1 = 1$) and near the bottom boundary were fixed to be cold ($\theta_0 = 0$).

By performing shear flow simulations using Lees-Edwards boundary conditions [6], we are able to calculate the particle-phase stress tensor σ, and the heat flux q [W/m²] (i.e., the sum of conductive, q^{cond}, and convective flux, q^{conv}) directly from the particle information. To make the heat flux dimensionless, we define q_s (Eqn. 5) as the reference conductive heat flux in the solid material the particles are made of.

$$\sigma = \frac{1}{V}\sum_i \left[\sum_{j\neq 1} \frac{1}{2} r_{ij} \otimes F_{ij} + m_i v_i' \otimes v_i'\right] \qquad p_c = \left(\sigma_{c_{xx}} + \sigma_{c_{yy}} + \sigma_{c_{zz}}\right)/3 \qquad (3)$$

$$q^{cond} = \frac{1}{V}\sum_c Q_{tot} r_{ij} \qquad (4,5)$$

$$q_s = -K \nabla_y T \qquad (5)$$

Results

As the particles are sheared in the x-(i.e., streamwise) direction, the particles collide with each other, exchange heat, and a linear (mean) temperature profile develops. The instantaneous conductive heat flux is calculated using Eqn. 4, and finally time averaged. Similarly, a time-averaged contact pressure p_c [N/m^2] between the particles is calculated using Eqn. 3. Here V is the box volume, r_{ij} is the center-center contact vector, and v' is the particle velocity fluctuation. Various validation tests have been performed, e.g., we have checked that the pressure calculated by us is in agreement with the data of Chialvo et al. [1]. Some of our results are summarized in Fig 2, illustrating the complex features of heat conduction in a granular material.

Fig 3 shows our results for the correlation of the contact pressure and the conductive heat flux. Clearly, there is a linear relationship between these two quantities. Surprisingly, this linear relationship (m is the slope) is independent of *Pe*, despite the fact that the temperature distribution is very different for different Peclet numbers (see Figure 2a).

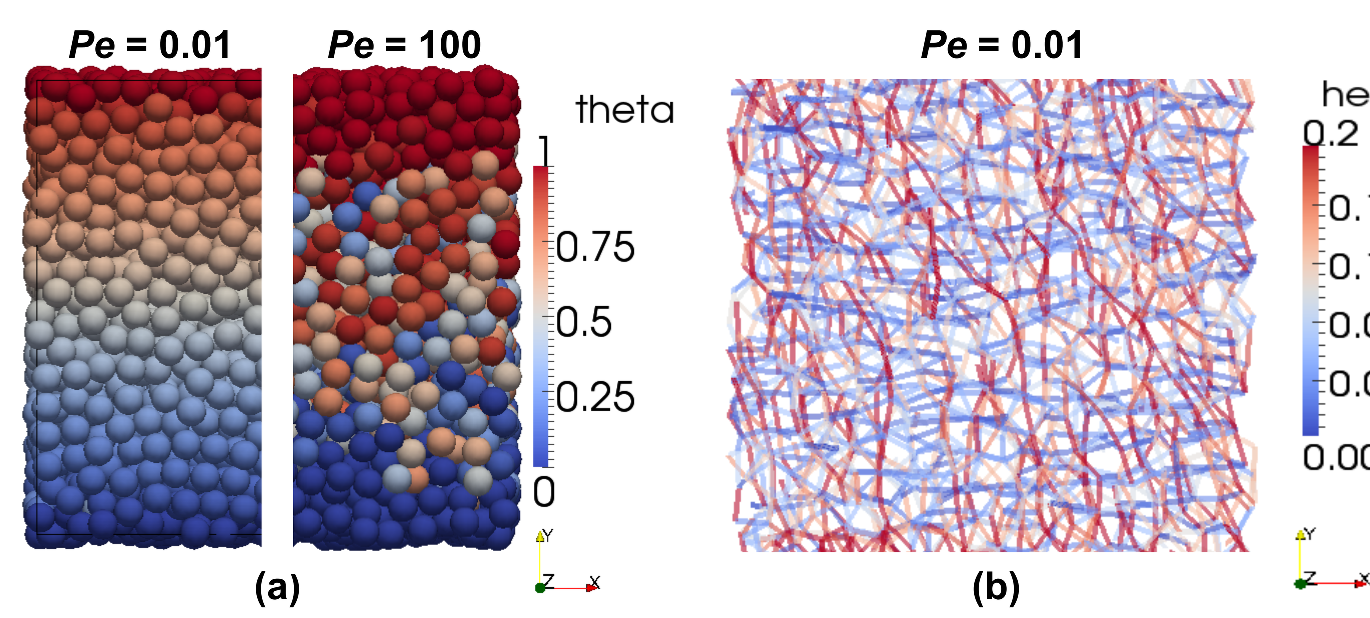

Fig. 2: (a) Snapshot of the particle temperature distribution, and (b) snapshot of the heat flux network between the particles (Φ_p = 0.59).

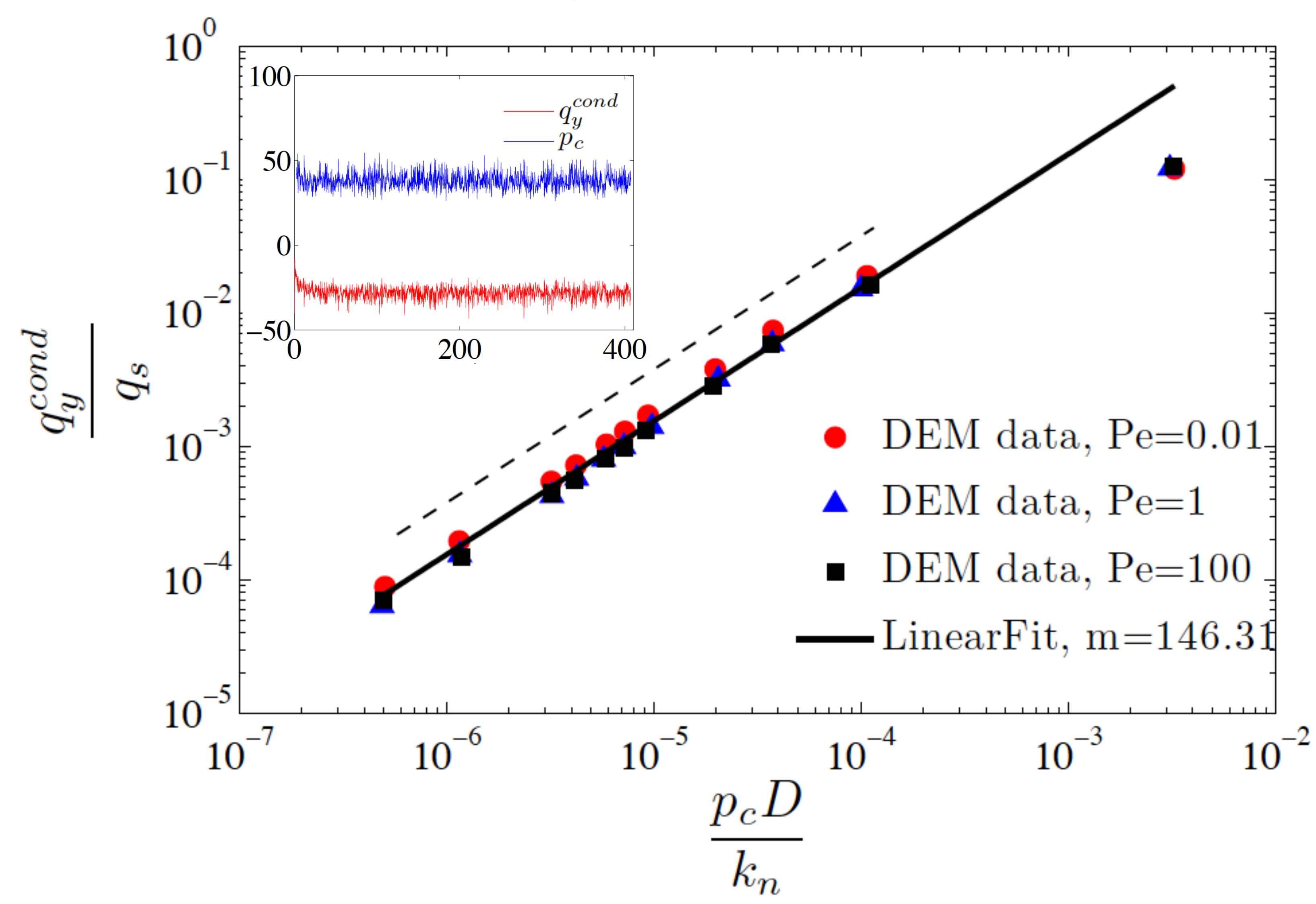

Fig. 3: Scaled conductive heat flux in the gradient direction vs. the scaled contact pressure for *Pe* = 0.01, 1.0 and 100 (points indicate results for different particle volume fractions; the inset shows the temporal fluctuations of the pressure and the conductive flux for Φ_p = 0.59 and *Pe* = 0.01).

Analysis and Proposed Model Structure

Assuming that the contact pressure is build up by normal contact forces only, one can readily derive the following relationships (here Z and $\Delta q'$ are the coordination number and the dimensionless particle temperature fluctuation, σ_c* is made dimensionless with k_n/D):

$$q^{cond*} \propto \phi_p \langle Z\rangle \left\langle \delta_c \left(1+\Delta\theta'\right) r_{ij}\right\rangle; \quad \sigma_c^* \propto \phi_p \langle Z\rangle \left\langle \delta_c r_{ij} \otimes r_{ij}\right\rangle \qquad (6)$$

Thus, in a regime where the particle-particle friction coefficient is unimportant, we expect a linear relationship between σ_c^* and q^{cond*}. In a more dense flow regime, this scaling is expected to break down, as indicated by our simulations.

Acknowledgement
This research was funded by the Austrian Science Foundation FWF (www.fwf.ac.at).

References
[1] S. Chialvo, J. Sun, S. Sundaresan, Bridging the rheology of granular flows in three regimes, Physical Review E. 85 (2012).
[2] P. Rognon, I. Einav, Thermal Transients and Convective Particle Motion in Dense Granular Materials, Physical Review Letters 105 (2010).
[3] P. Rognon, I. Einav, J. Bonivin, T. Miller, A scaling law for heat conductivity in sheared granular materials, Europhysics Letters 89 (2010).
[4] C. Kloss, C. Goniva, A. Hager, S. Amberger, S. Pirker, Models, algorithms and validation for open source DEM and CFD–DEM, Progress in Computational Fluid Dynamics 12 (2012) 140–152.
[5] P.A. Cundall, O.D.L. Strack, A discrete numerical model for granular assemblies, Geotechnique 29 (1979) 47–65.
[6] A. Lees, S. Edwards, The computer study of transport processes under extreme conditions, Journal of Physics C: Solid State Physics 1921 (2001).