THERMAL CONDUCTIVITY OF 2D RANDOM INTERFACES

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Abstract. Heat transfer through dense granular interfaces formed by squares or triangles with randomly assigned thermal conductivities is discussed. The effective thermal conductivities of the interface are found by means of the steady heat flux induced by connection of interface with the external heat source assuring the constant value of boundary temperature. Some statistical properties of effective conductivities are also presented.

Introduction

In many situations of engineering and applied mathematics interest one is confronted with energy transport in heterogeneous medium. Especially, transport phenomena within granular media, such as sound propagation, heat transfer or electrical conduction, are of great industrial importance. They display many astonishing properties such as slow relaxations, stochastic current fluctuations, percolation. These properties can be due to the extreme sensitivity of the inter-grain interactions to details of granular packing and to the nature of the grain surface. The microstructure of a granular medium is the main feature that makes these heterogeneous materials different from their homogeneous counterparts. For granular materials the magnitude of effective conductivity depends on the surface roughness, the type of material, and the interface pressure [1-3].

Numerous researches in the area of granular heat transfer, use the effective medium approximation (EMA). This approach provided accurate solutions of steady, averaged temperature profiles using detailed characterization of the microstructure [4]. Within EMA, the heat transport through a heterogeneous medium can be expressed via classical continuum relation

\[ c(T) \frac{\partial T}{\partial t} = \lambda_{eff} \nabla^2 T \] (1)

The mean system’s temperature is \( T \) and \( \lambda_{eff} \) is the so-called effective thermal conductivity, \( c(T) \) is the volumetric specific heat. Equation (1) represents a kind of operational point of view when a system is considered as a black box whose input and output are characterized by different temperatures and \( \lambda_{eff} \) aggregates all local information about the sample details. In this concept \( \lambda_{eff} \) reveals an ability to the
heat propagation with no macroscopic mass transfer. For 1D system of length $L$ and cross-section $A$, the thermal conductivity can be defined by means of the stationary flux $q$ of energy $Q = A J$, induced by connection of the system to thermostats assuring the temperature difference equals $\Delta T$. This energy flux is proportional to $\Delta T$ and its value is expressed by the formula

$$Q(L, \Delta T) = \lambda_L \Delta T \frac{A}{L}$$  \hspace{1cm} (2)

For finite $\lim_{L \to \infty} \lim_{\Delta T \to 0} \lambda_L < \infty$, we have the normal conductivity and the system satisfies the Fourier law. Thus the effective thermal conductivity is given by the following expression

$$\lambda_{\text{eff}} = \lim_{L \to \infty} \lim_{\Delta T \to 0} \lambda_L = \psi(\text{geometry and material details}) \cdot \frac{q}{\Delta T}$$  \hspace{1cm} (3)

In a case of the simplest geometry one obtains

$$\psi = \frac{L}{A} \quad \Rightarrow \quad \lambda_{\text{eff}} = \frac{L}{A} \cdot \frac{Q}{\Delta T}$$  \hspace{1cm} (4)

where: $Q$ is the amount of heat transmitted in a direction perpendicular to the surface $A$ due to the temperature difference $\Delta T$. Here, the steady heat flow is assumed, of course.

An ensemble of geometrically identical grains with random transport capabilities yields the effective transport properties of whole grain ensemble highly dependent on details of the arrangement of the grains’ collection. The influence of particle shape on heat propagation through a granular medium in the state of random packing is discussed. We use Thermal Particle Dynamics (TPD) simulation technique which allows to compute transport properties of granular system under static condition [5]. The main advantage of TPD is that by incorporating contact conductance theories simultaneous two-body interactions may be used to model the heat transfer in a system composed of many particles.

Here an example of two dimensional granular interface formed by identical squares or by equilateral triangles is considered (see Fig. 1). For each of these shapes the grains are characterised by the thermal conductivity coefficient $\lambda$, taken to be random with two-point distribution function.

Fig. 1. Granular system consists of equilateral triangles, two colours correspond to two different values of the thermal conductivity coefficients of $\lambda$. The values of $\lambda$ are assigned randomly
1. Mathematical formulation of the problem

The system is structurally heterogeneous with respect to the thermal conductivity coefficients.

\[
\begin{align*}
\left( \frac{\partial^2 T}{\partial x^2} \right)_{i,j} + \sum_{k=1}^{N} \alpha \left( \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{h^2} \right) + \sum_{l=1}^{N} \beta \left( \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{h^2} \right) &= 0
\end{align*}
\]

(5)

where the curly bracket emphasises the stochastic nature of thermal conductivities.

An effective thermal conductivity \( \lambda_{\text{eff}} \) is the global property of the material which reveals an ability to heat conduction with no need of any macroscopic mass transfer. The effective thermal coefficient is computed using the Equation (3), within a statistical ensemble of grain arrays with randomly distributed values of \( \lambda \). In this statistical approach an estimated value of \( \lambda_{\text{eff}} \) is the mean value of the probability distribution of \( \lambda_{\text{eff}} \) numerically computed for an ample set of samples

\[
\lambda_{\text{eff}} = \frac{1}{N} \sum_{i=1}^{N} \left( \lambda_{\text{eff}} \right)_{i,j} = \frac{1}{N\Delta T} \sum_{i=1}^{N} \psi(\{\lambda\}_{i})Q
\]

(6)
where $\psi(\{\lambda\})$ represents the particular realisation of $\lambda$ distribution within the one member of the statistical ensemble.

**2. Examples of numerical calculations**

Two numerical experiments: with square-shaped and triangle-shaped grains have been realized. For each of this experiments we constructed the macroscopic samples using about 50×50 grains with randomly assigned values of $\lambda$ and we computed the corresponding $\lambda_{\text{eff}}$ according to the Eq. (3). Thus, for these two geometries we obtained statistical ensembles, each with about $10^5$ samples for all values of $p = 0.1, 0.2, ..., 0.9$, where $p$ is the parameter defining the random two-point distribution of $\lambda$. Figure 3 shows one of the member of statistical ensemble for square-shaped grains and the distribution of the temperature within the macroscopic sample when the steady state is attained.

Fig. 3. Square-shaped grains with $\lambda = 5$ and $\lambda = 1$ form the macroscopic sample. Temperature distributions correspond to: $p(\lambda = 5) = 0.4, 0.6$ and 0.8
The corresponding probability density $P(\lambda_{\text{eff}})$ is presented in Figure 4. This is the normal distribution centered at $\lambda_{\text{eff}} = 0.65$.

![Figure 4](image)

Fig. 4. Probability density $P(\lambda_{\text{eff}})$ for an array of 50×50 square grains with random values of $\lambda_1 = 1$ and $\lambda_2 = 5$, and $p(\lambda_2) = 0.4$. $\lambda_{\text{eff}}$ is computed with $5 \cdot 10^5$ samples.

We have computed the mean values $\lambda_{\text{eff}}$ according to Equation (5) and the corresponding distribution is presented in Figure 5.

![Figure 5](image)

Fig. 5. $(\lambda_{\text{eff}} - p)$ curve for square-shaped (squares, c) and triangle-shaped (triangle) arrays of about 50×50 grains with random values of $\lambda_1 = 0.2$ and $\lambda_2 = 2.0$. Points correspond to the values of $\lambda_{\text{eff}}$ averaged over $10^5$ samples.
Conclusion

In this paper we have reported results of the EMA approach to the heat transfer through the interfaces formed by mixtures of microscopic grains with randomly assigned “microscopic” thermal conductivities. We have analysed numerically two types of interfaces: consisting of the densely packed square-shaped grains only and these with the triangular grains exclusively. We have also assumed the perfect inter-grains heat contact. The obtained distributions of the effective thermal coefficient does not depend visibly on the grains’ shapes. This is due to the perfect grains’ packing of an ample number of grains. In such circumstances the randomness is introduced only by variation of the grains “microscopic” characteristics and thus the system behaves as the collection of point-like objects. The shape of grains will play a pronounced role if we introduce another phase to the system apart the solid state grains’ phase. This can be achieved e.g. by introducing the liquid or gaseous medium between the grains.

References