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Modeling of granular packed beds, their statistical analyses and evaluation of effective thermal conductivity

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ABSTRACT

Thermal conductivity of packed beds plays the key role in the emerging technologies of selective laser melting/sintering. The objective is to study the influence of the packed bed structure on the contact thermal conductivity. The discrete (network) model of the contact thermal conductivity in the packed particle layer is proposed. The task of heat transfer due to the contact thermal conductivity of the system of parallel the located cylinders with the fixed thermal resistance of the contact is solved in the 2D case. The 3D-task on the heat transfer through the layer of spherical particles of finite thickness in between heated solid massive bodies with constant and different temperatures is solved. In the calculations, the package structures were varied: the regular (with the cubic symmetry), random (with the mono- and poly-disperse particles), as well as the porosity and mean coordination number. The effective thermal conductivity coefficient was evaluated as the packed bed structure, the mean porosity, and coordination number were varied. The calculation results agree with the known analytical solutions. The statistical analysis of regular and packed beds of solid spheres is presented.

1. Introduction

Thermal conductivity in packed beds (PBs) of loose powder is very important in such technological processes as selective laser melting (SLM) or selective laser sintering (SLS) of powders. In these processes, a thin powder layer is put on a substrate, and a laser beam sequentially scans the surface of the powder layer, which leads to fusion or sintering of the treated powder particles. The laser scanning is repeated many times until a complex part is built. Note that in these processes, spheroidized powders are preferable. Nonuniformity of the thermal action on the powder surface results in the development of high temperature gradients concentrated in local areas. In this case, the mechanisms of heat transfer in the powder bed are of great interest. At present, there are many theoretical models for predicting the structure of PBs of spherical particles and calculating heat transfer in such media. The next section reviews these models.

1.1. *Modeling the structure of packed beds of spherical particles*

When simulating the PBs of monodispersed particles within the range from 1 to 1000 μm [1], the discrete element method was used; it considers the mechanisms of interaction of the particles with each other, with due regard to rotation and elastic properties of the particle material. The momentum and angular momentum equations include, the normal and tangential components of the contact force between particles, the gravity force and the Van der Waals force describing adhesion among particles.

The discrete element method [2] is the best to model the physics of contact interaction between particles. To model the structure of a packed bed, the simultaneous motion of all the particles should be calculated. This may result in the overestimation of density in the PB compared to the observed density of loose power. The generated packed beds were analyzed using the Voronoi-Delaunay mosaic theory [2].

The authors [3] proposed a simple algorithm of sphere packing in a cubic case based on consequent dropping of the spheres and their deposition under the action of the gravity force. The initial coordinates of the particles were randomly generated. Only elastic

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Nomenclature

t	time
x, y, z	coordinates
k_i	number of contacts of $i-$ particle
l	linear size
r	radius
c_s	specific heat capacity
$R_{ij}, \widehat{R}_{ij}$	specific spreading resistance
n	number density of particles
u	specific conductance of a contact in 2D
s	conductance of a contact in 3D
T	temperature, K
a_{ij}	radius of the contact
A_{eff}, K_{eff}	effective thermal conductivities
D	diameter of the TE
M	number of particles
N	mean coordination number
Q	heat fluxes, power
q_{ij}	amount of heat transferred per time unit through each contact
α_{ij}	the angular radius between TEs
ϕ	azimuthal angle
ε	porosity
λ_{pi}	thermal conductivity of particle material
ν	angular distribution
θ	polar angle
ρ	density

Subscripts

p	particle
x, y, z	coordinates
s	solid

Abbreviations

PB	packed bed
TE	thermal element
SLM	selective laser melting
SLS	selective laser sintering

interaction of the particles was considered. Each sphere was stopped and stayed in the position where the gravity force was balanced by the repulsion elastic forces of the previously deposited spheres. The presence of elastic forces at the particle collision imitated the system bumping-down, which violates the condition of the loose packing.

Al-Raoush and Alsaleh [4] constructed the PB of the poly- and monodisperse solid spheres in accordance with the algorithm of the random choice of initial sphere coordinates inside a hexahedral area, with due regard to the mean coordination number of the PB. The new sphere was added to the previously placed ones, and moved toward the chosen target sphere in accordance with the coordination number obtained from the density distribution taken from micrographs of the experimental sample. Optimization of the constructed PB involves isotropy, uniformity, and chaotic character of the solid sphere system. It was carried out by the sequential quadratic programming method.

Corwin et al. [5] developed the model of random packing of polydisperse spheres with no regard to friction. This model was applied to describe geometrical properties of emulsions. The model permits calculating the distribution of the nearest neighbors, the positions of contacts and local compactness fluctuations, along with the global compactness of the PB.

In this study, we used the method of calculation of the structure of the PB of mono- or polydisperse spherical particles [6]. The method gives the structure of the PB, which closely approached loose packing without compacting. The coordinates of the particle mass center in the PB were found after the random gravity-driven drop of individual spheres on the substrate or in a representative volume. The non-elastic collision of the spheres and their adhesion interaction were taken into account, which permitted simulating loose powder beds with various porosities owing to the variation of the physical properties and the sizes of particles. Appendix A presents the mathematical problem statement and the solution algorithm.

1.2. Modeling heat transfer in the system of contacting particles

Effective thermal conductivity in the system of packed contacting particles is considered as an important property. The known models of heat transfer in granular or porous media consider the phenomena of the contact or network heat transfer in order to obtain approximative dependences for the effective thermal conductivity [7,8]. The effective thermal conductivity depends on the number of parameters describing the PB structure. To obtain the effective thermal conductivity, the most of the models consider heat transfer in the representative volume of the granular medium. In the number of works, the analyses are carried out in the representative container filled with the granular medium consisting of elementary cells. Each cell of such a medium includes a selected particle surrounded by the neighboring particles contacting it. In the cell, heat is transferred by two parallel channels: through the cavities filled with a fluid, and through the solid phase.

Cheng et al. [9] proposed the method for evaluating the effective thermal conductivity of the PB of monodispersed spheres neglecting the convection of fluid in pores; the method is based on the conductivity through solid particles and through fluid gaps between non-contacting particles. It requires the information on

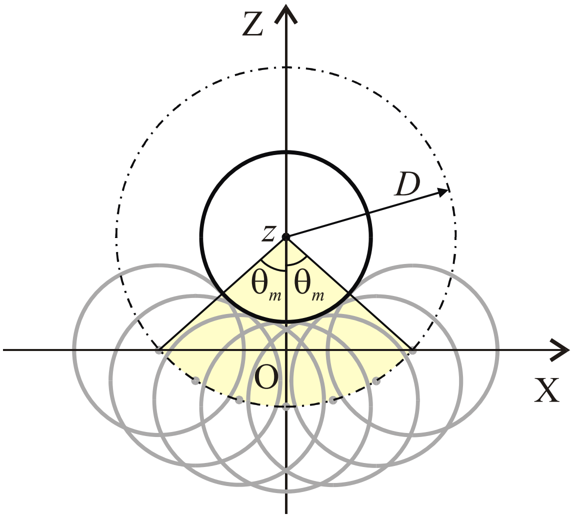

Fig. 1. Possible pairs of contacting particles contributing to heat transfer through plane $z = 0$.