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Efficient method for predicting the effective thermal conductivity of various types of two-component heterogeneous materials

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ABSTRACT

A new method for modelling the effective thermal conductivity of a two-component heterogeneous material is proposed. The model is intended to apply, in general, for any thermal conductivity ratio (K) between the two components, and for any geometry in which the higher conductivity material forms at least one continuous pathway. The model combines the resistances for the energy carriers inside the continuous path in $K \to \infty$ and $K \to 1$ regimes in a novel way. As a result, the modelling of complex geometries becomes possible with reasonable efforts. The validity of the model was tested with six different basic geometric structures ranging from closed cell structures to randomly oriented fibers. By variating aspect ratios and volume fractions of the basic structures, in overall 43 different geometrical cases were analyzed, all within thermal conductivity ratio range $1.2 \leq K \leq 40000$. Typically, the standard mixing rules and models do not sufficiently take into account the change in direction of energy carriers when conductivity ratio K is altered. As a result of this, it was found that these models are usually valid only within the range $K \leq 4$. For almost all structures the overall performance of the new model was instead significantly better. An exception was the Kelvin foam structure for which the new model and Maxwell equation resulted in an accuracy of the same order of magnitude.

1. Introduction

Modelling of thermal conductivity of composites, colloids and other heterogeneous materials is important for various applications such as thermal insulation [1–3], thermal barrier coatings [4], PCM storages based on composites and mixtures [5–7] and drying.

The classical general models for the effective thermal conductivity, such as the Maxwell's equation (equal to Hashin-Shtrikman bounds), Hamilton-Crosser equation [8] and methods of combining parallel and serial resistances [9] have been shown to perform for special cases with a reasonable accuracy. Based on correlations, the Maxwell's equation has been extended for open-cell foams by introducing an effective solid phase tortuosity [10]. Some authors [11] have combined different general models developing a unifying model that does not take into account the actual structure of the material. Models with adjustable parameters have been suggested [12] as well. Most typically the models are dedicated to certain applications, geometries and materials such as wood (e.g. wood briquettes [13]). Recently, a quasi-periodic field method for the numerical evaluation of the effective conductivity was also developed [14].

The objective of present study is to find a method for modelling heterogeneous materials that is applicable for various types of geometries and for any conductivity ratio

$$K = \frac{k_H}{k_L} \tag{1}$$

where material H has higher conductivity than material L ($k_H \geq k_L$). The main geometrical restriction of present model is that material H has to form at least one continuous path between the heat transferring boundaries. However, part of the material H can appear in a dispersed phase as well. The material L can form dispersed, continuous or a combination of dispersed and continuous sections. The conductivity ratio K determines the path of energy carriers (phonons and free electrons) inside the material. Based on computer simulations, the effect of K is illustrated in Fig. 1. For small values of K (Fig. 1a) heat flows almost straightforwardly from the bottom to the top. When the conductivity ratio increases the movement is oriented more and more to the material H. Finally, with a very high ratio (Fig. 1d) heat principally conducts only through the tortuous continuous path of material H. It should be noted that high values of K can be reached also for a low conductivity solid materials H if material L is in a gas phase. The gas conductivity can be very small if the pressure is very low (see e.g. the effect on silica aerogel insulators in Ref. [15]). If L is in vacuum, then $K \to \infty$. The decrease in conductivity can be detected also if the gas is

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Nomenclature

a, b, d, l, h, s	size (meaning of the symbol depends on the structure), m
A	cross-sectional area, m^2
D	distance between two opposite faces of a tetrakaidecahedron, m
ER	model error, %
f	volume fraction
G	dimensionless factor
k	thermal conductivity, $Wm^{-1}K^{-1}$
k_{eff}	effective thermal conductivity, $Wm^{-1}K^{-1}$
K	$= \frac{k_H}{k_L}$,
r	aspect ratio
R	thermal resistance, KW^{-1} (three-dimensional), mKW^{-1} (two-dimensional)
T	temperature, °C
W	width, m
Y	depth, m
Z	length (in direction to the main heat flow), m

Subscripts

branch	fraction of the higher conductivity material that is not accounted for the continuous path
C	continuous phase
D	dispersed phase
H	material with higher conductivity
HD	material *H* in dispersed phase
L	material with lower conductivity
p	particle
tot	total
1	phase 1
2	phase 2

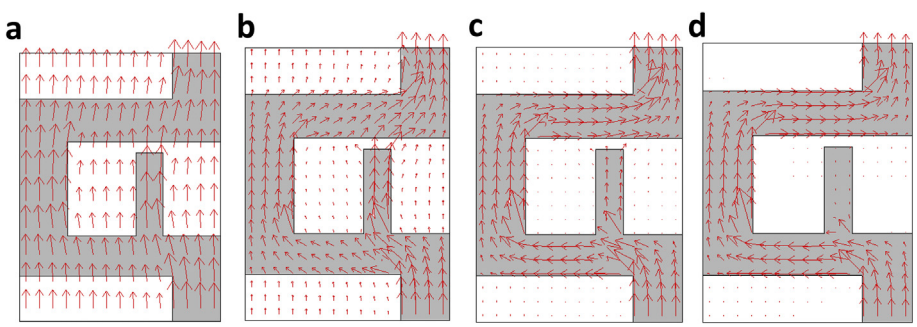

Fig. 1. Heat flow vectors in a two-dimensional structure. Darker sections are composed of material *H* and lighter of material *L*. Vertical boundaries are treated with a symmetry condition. a) $K = 2$, b) $K = 10$, c) $K = 100$, d) $K = 1000$. The vectors are numerically solved from the heat equation (for methods, see the end of Section 2.2).

Table 1
Summary of geometries.

Structure	Aspect ratio	f_L	f_{branch}
2D concentric rectangles	$b/a = 1/2$ [a]	0.16, 0.36, 0.58, 0.77, 0.92, 0.988	no branches
	1	0.16, 0.36, 0.58, 0.77, 0.98	no branches
	2 [a]	0.18, 0.41, 0.58, 0.76, 0.99	no branches
2D tree structure	$b/s = 3.5$	0.42	0.22
	9.3	0.80	0.28
	24	0.93	0.30
	117	0.986	0.31
2D randomly oriented fibers	$l/s = 10$	0.964	0.38 (4 resistances for R_1), 0.48 (14 resistances for R_1)
3D concentric cuboids	$d/h = 1$	0.50, 0.73, 0.89, 0.97	no branches
	2.3 [a]	0.39, 0.73, 0.89, 0.97	no branches
3D Kelvin foam structure		0.25, 0.51, 0.75, 0.89, 0.95	0.13, 0.11, 0.057, 0.019, 0.0065
3D tree structure	$l/d = 2.2$	0.73	0.17
	4.5	0.80	0.32
	9.5	0.89	0.38
	19.5	0.95	0.38
	50.2	0.994	0.41
	19.5	0.95	0, 0.18, 0.43, 0.64

[a] Aspect ratio of the inner rectangle or cuboid.

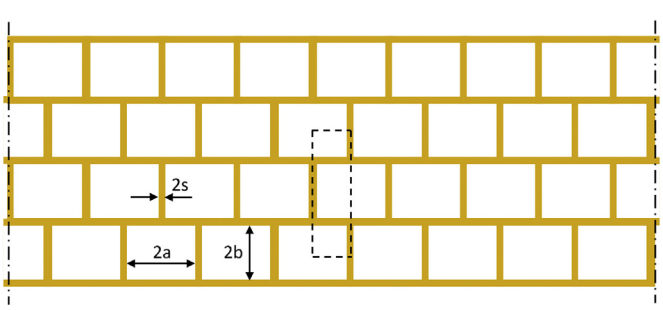

Fig. 2. A composite of concentric rectangles.

trapped inside micro- or even nanosized gaps. Therefore, the change in direction of energy carriers in Fig. 1 can be observed either by reducing the pressure of gas, or changing the structure size from macroscale to nanoscale. Except for certain specific geometries and for a limited *K* range, the change in energy carrier movement is poorly accounted for in standard mixing rules and models. The model developed in the present work aims to solve this particular problem.