

Calculations of the Thermal Conductivity of Porous Materials

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Abstract. In this paper, the geometrical effective thermal conductivity of porous materials is investigated based on two different approaches: the finite element method as a representative for numerical approximation methods and an analytical method for 2D homogenised models based on a solution of the respective boundary value problem. It is found that the relative conductivity is practically independent of the specific shape or topology of the inclusions. Only the morphology (closed-cell or open-cell) of the structure slightly influences the conductivity. Furthermore, it is shown that a small perturbation of the circular inclusions of 2D models increases the effective conductivity.

Introduction

Porous metals exhibit particular physical and mechanical properties that differ highly from classical full dense materials. Interesting combinations of these properties, such as high thermal conductivity combined with high gas permeability or relatively high stiffness in conjunction with very low specific weight, offer the possibility for new future-oriented multifunctional applications, e.g. cooling and heating systems, heat exchangers or fire protection. The most important structural parameters which characterise a cellular metal are the morphology of the cell (geometry, open or closed cell), the topology, the mean cell size and the relative density $\rho_{\text{rel}} = \rho/\rho_s$ (the macroscopic density, ρ , divided by that of the solid material of the cell wall, ρ_s).

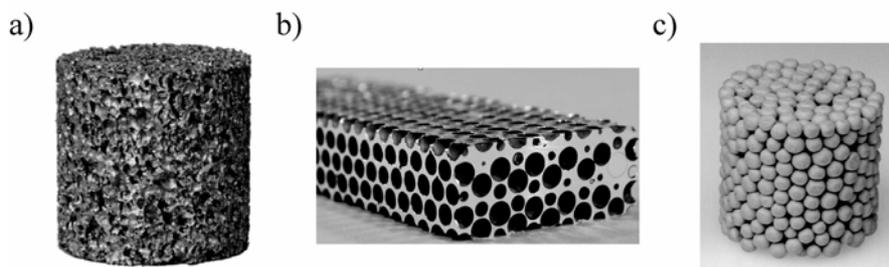


Figure 1. Different types of porous materials: a) closed-cell metal foam (ALPORAS®); b) hollow alumina spheres embedded in a magnesium matrix [1]; c) hollow sphere foam Fe_{0.88}Cr_{0.12} [1].

In this paper, the geometrical effective thermal conductivity of porous metals based on conduction in the solid material is investigated. Two different methods, namely a numerical and an analytical approach, are applied. The finite element method allows for consideration of arbitrary pore geometries and nonlinearities (e.g. material or boundary conditions). However, the numerical approach is in many cases restricted to the consideration of a single unit cell or periodic structures in order to reduce the computation time. The analytical approach allows for an easy consideration of perturbations in the pore arrangement. Results obtained from both approaches are presented and compared.

Finite Element Approach

The numerical investigation of the relative thermal conductivity $\lambda_{\text{rel}} = \lambda/\lambda_s$ (λ is the effective conductivity of the porous material and λ_s the conductivity of the solid material) is performed with the commercial finite element (FE) code MSC.Marc. The basic idea of the finite element method is the decomposition of a domain with a complicated geometry into geometrically simple elements, such that the governing differential equation can be solved (approximately) for these finite elements. The single element solutions are then assembled to obtain the complete system solution using given boundary conditions. The assembly process uses appropriate balance equations at the nodes which are used to define the elements and serve also as connection points between the elements. In the scope of this study, different 2D and 3D structures are investigated (cf. Fig. 2). According to [2,3], the influence of radiation inside the pores can be neglected. Furthermore, the thermal conductivity of included media (e.g. air, $\lambda_1 \approx 0.025\text{W}/(\text{m}\cdot\text{K})$, [4]) is typically several orders of magnitudes smaller than the cell wall material (e.g. aluminium $\lambda_s = 221\text{W}/(\text{m}\cdot\text{K})$, [4]). Beyond, in compliance with [5] heat transfer due to convection of gaseous media in the pores of closed cell foams with small cell size can be disregarded. However, a significant contribution of the heat flux due to convection can be expected for open-cell structures. In order to maintain the comparability of the results, convection has therefore been disregarded. Accordingly, inclusions can be approximated as voids with no contribution to the thermal conductivity of the structure ($\lambda_1 = 0$). Consequently, only the thermal conduction in the base material λ_s is considered for our basic studies and only the geometry of the structure has to be modelled.

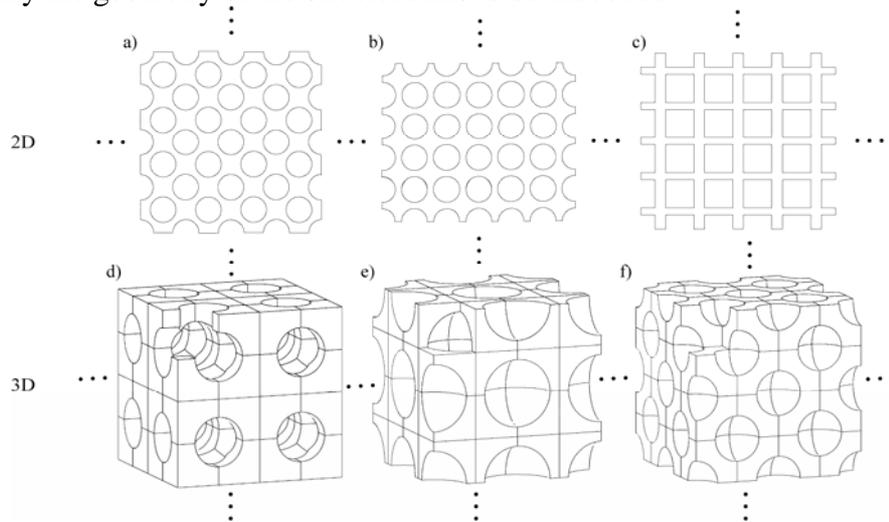


Figure 2. Representative areas/volumes: a) circular 45° , b) circular 0° , c) squared, d) open-cell, e) spherical body-centered cubic (bcc), f) spherical face-centered cubic (fcc).

The relative density ρ_{rel} of the illustrated geometries is varied by modification of the distance of the inclusions, whereas their size remains constant. Since the available computer hardware limits the number of degrees of freedom, not the whole 2D or 3D structure can be meshed. Alternatively, only one fourth of the unit cell is modelled and specific symmetry boundary conditions ($\frac{dT}{dx} = \frac{dT}{dy} = \frac{dT}{dz} = 0$) are introduced on the surfaces outside the xz -planes (cf. Fig. 3, grey areas) in order to simulate the influence of the adjacent cells. Corresponding to Fig. 3, all FE models describe the thermal behaviour of an infinite structure, where the influence of a free boundary is disregarded. This homogenisation is accurate for structures that consist of more than 10 to 15 units cells in every direction. The number of nodes for the different meshes are summarised in Table 1.

Number of nodes as an indicator for the mesh density

ρ_{rel}	3D open cell	3D fcc	3D bcc	2D circular (45°)	2D circular (0°)	2D square
0.1	14329	-	-	-	-	-
0.2	19197	-	-	-	-	-
0.3	19960	-	-	1649	-	-
0.4	20207	-	-	4009	-	-
0.5	17435	42385	55281	5377	26499	26499
0.6	28532	42385	37640	6527	23137	23137
0.7	28485	29797	24217	1643	14991	14991
0.8	35515	29797	24217	1233	9387	9387
0.9	32249	16249	14436	1507	17013	17013
0.95	-	16249	7721	-	22057	22057

Table 1. Mesh density for different configurations

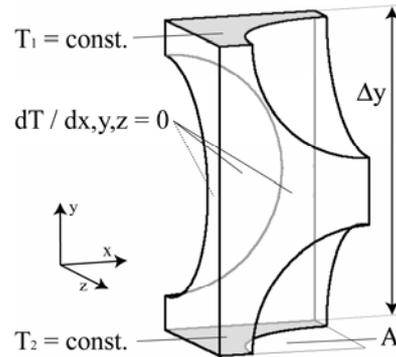


Figure 3. Boundary conditions in the case of the 3D spherical bcc model.

Since the cross sectional Area A and the spatial distance Δy are defined by the geometry, respectively the gradient $\nabla T = T_2 - T_1$ by the boundary conditions (cf. Fig. 3), only the heat flux \mathcal{Q} remains to be determined. This is done by summing up all nodal values i of the ‘reaction heat flux’ at the top or bottom line (2D) / surface (3D) where a temperature boundary condition is prescribed:

$$\mathcal{Q} = \sum_i \mathcal{Q}_i \quad (1)$$

Analytical Approach

A composite material with periodically placed cells with random inclusions inside is considered within the analytical approach. Based on an unit cell representing the whole composite [6,7], corresponding values of the effective conductivity are approximately derived under the assumption that the inclusions can be treated as empty pores with the conductivity $\lambda_1 \rightarrow 0$. For this approach, 2D composite materials with periodic and quasi periodic structures (i.e. periodically located cells containing a finite number of random non-overlapping circular inclusions) are considered (cf. Fig. 4).

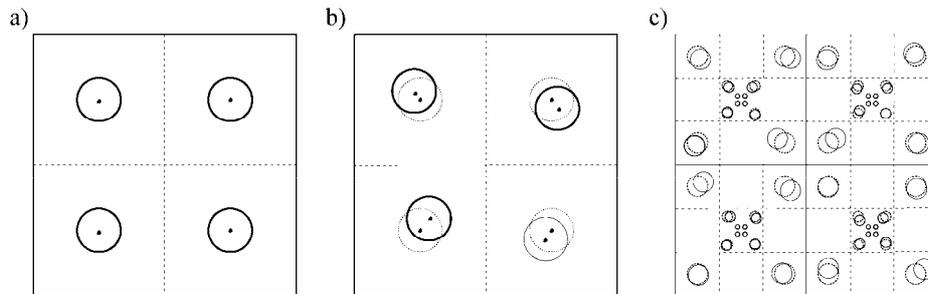


Figure 4. a) Periodic square array of inclusions; b) perturbed array of inclusions; c) periodic and perturbed pseudofractal array of inclusions.

In the framework of this approach, conductive properties of composite materials can be described in terms of conjugation conditions $u^+ = u^-$, $\lambda_s \frac{\partial u^+}{\partial n} = \lambda_1 \frac{\partial u^-}{\partial n}$ on the boundary of inclusions ∂D_k with

respect to the function $u(x, y)$ (e.g. the temperature) sectionally harmonic in D^+ and D^- [6,7]. These conjugation conditions correspond to a perfect contact between different materials. Here, D_k are simply connected domains modelling inclusions of conductivity λ_1 in the matrix material D^+ of conductivity λ_s , $D^- := \bigcup_{k=1}^N D_k$. If the field is potential, i.e. the function $u(x, y)$ satisfies the Laplace equation $\nabla^2 u = 0$ in a domain D , then one can introduce the function $\varphi(z) = u(z) + \imath v(z)$, $z = x + \imath y$, $\imath^2 = -1$, analytic in D which is called the complex potential and reformulate the problem in terms of this potential.

The effective conductivity of macroscopically isotropic composite materials with small concentration ν of nonrandom inclusions is described by the classical Clausius-Mossotti formula (for background and application see [8])

$$\lambda_{\text{rel}} = \frac{\lambda}{\lambda_s} = \frac{1 + \mu\nu}{1 - \mu\nu}, \quad (2)$$

where $0 < \lambda_s < +\infty$ is the conductivity of the matrix and $\mu = \frac{\lambda_1 - \lambda_s}{\lambda_1 + \lambda_s} \in [-1, 1]$ is the contrast parameter which expresses the difference between the conductivity of both materials.

The generalisation of this formula for quasi periodic composites with random inclusions of the conductivity $\lambda_1 > 0$ is obtained in [6] as:

$$\frac{\lambda}{\lambda_s} = 1 + \frac{2\mu\nu}{N} \sum_{m=1}^N \psi_m(a_m), \quad (3)$$

where $\nu = N\pi r^2$ is the concentration of inclusions which can be expressed in the case of a simple cell of unit size as $\nu = 1 - \rho_{\text{rel}}$. Variable r is the radius of inclusions, N is the number of inclusions in the cell, a_m are the centres of the inclusions and $\psi_m(z)$ are the derivatives of complex potentials in the cell. The sum on the right hand side of the Eq. 3 is reduced to a power series approximation with respect to ρ_{rel} :

$$\frac{\lambda}{\lambda_s} = 1 + 2\mu(1 - \rho_{\text{rel}})[A_0 + A_1(1 - \rho_{\text{rel}}) + A_2(1 - \rho_{\text{rel}})^2 + A_3(1 - \rho_{\text{rel}})^3 + \dots]. \quad (4)$$

The coefficients A_p can be found for square and pseudofractal arrays of inclusions in [9]. A square array of inclusions refers to their distribution for which the centres of the inclusions form a square (cf. Fig. 4a). It is shown in [6,9] that random perturbation of the inclusions of square (cf. Fig. 4b) and pseudofractal (cf. Fig. 4c) arrays increases the effective conductivity of a composite under the requirement that each inclusion is moved in such a way that it cannot touch or cross with others. Thus, periodic square and periodic pseudofractal arrays of circular inclusions provide a minimum for the effective conductivity in the class of periodic macro-cells with random microstructure.

Results

The results of the FE analysis for the relative conductivity λ_{rel} are shown in Fig. 5a.

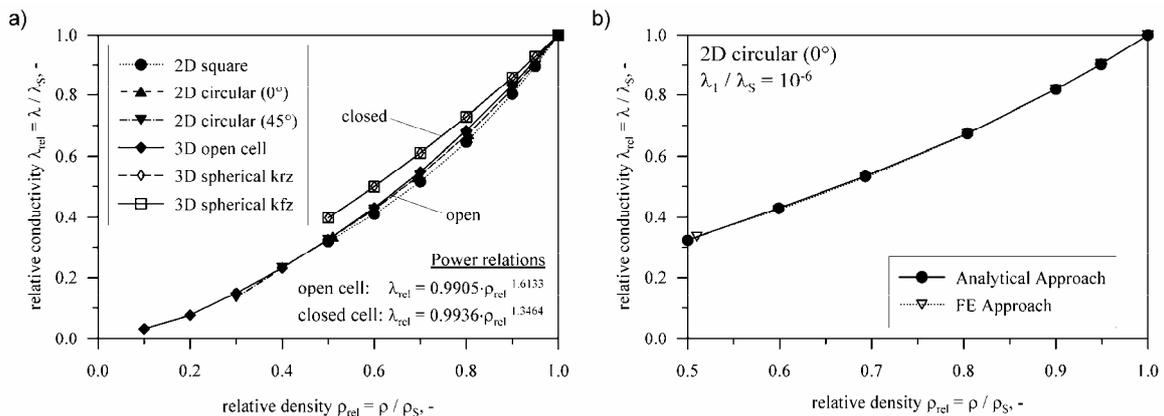


Figure 5. Relative conductivity λ_{rel} in dependence on the relative density ρ_{rel} .

The relative thermal conductivity λ_{rel} seems to be independent of the shape and the topology of the inclusions. Only the morphology of the structure influences the behaviour: the results for the two closed-cell structures (fcc and bcc) coincide at slightly higher values compared to the various open-cell geometries. However, the relative density ρ_{rel} seems to be an appropriate generalised parameter for a first description of the relative conductivity of porous materials. Therefore, power relations for open and closed cell structures are given in Fig. 5a. In Fig. 5b, the results of the analytical approach are compared with the numerical findings in the case of the 2D circular (0°) structure and a very good correlation is found. Furthermore, the effect of an increasing relative conductivity due to small perturbations is analytically verified. The maximum deviations of 0.36 and 0.45 % to the results of the unperturbed structures are determined for a relative densities of $\rho_{\text{rel}} = 0.7$, respectively $\rho_{\text{rel}} = 0.6$.

Conclusions

The relative thermal conductivity λ_{rel} is numerically determined for different structures (2D and 3D) as a function of the relative density ρ_{rel} . For the 2D circular (0°) structure, the results are independently obtained by means of a analytical approach and very good correlation between the two attempts can be observed. It is numerically shown that the relative conductivity seems to be practically independent of the specific shape or topology of the inclusions. Only the morphology (closed-cell or open-cell) of the structure shows a minor effect on λ_{rel} . Therefore, the parameter ρ_{rel} enables the estimation of the relative thermal conductivity of common porous materials (cf. Fig. 1). Furthermore, the increase of the effective conductivity for the 2D models under small perturbations is analytically proven.

Acknowledgements

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