

Analysis of thermal conduction in carbon foams

A.M. Druma, M.K. Alam*, C. Druma

Department of Mechanical Engineering, 251 Stocker Center, Ohio University, Athens, OH 45701, USA

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Abstract

Carbon foams are a new class of porous organic materials that are being developed for use as insulation, heat spreaders, and compact heat exchanger cores. The thermal conductivity of carbon foams is difficult to determine analytically, particularly for the case of high porosity, graphitic foams that show moderate to high bulk conductivity. Models that predict thermal conductivity of foams often use an empirical parameter to account for the effect of pore shape and material microstructure on the conduction process. A finite element (FEM) analysis has been developed to calculate the thermal conductivity of carbon foams for the complete range of porosity. The results are interpreted in terms of analytical and semi-empirical solutions. It is shown that the FEM solution matches the theoretical solution that is valid for low porosity, but differs significantly from semi-empirical solutions of high porosity foams.

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1. Introduction

Several multi-phase materials occur in nature and many are fabricated as engineered materials, such as composites and foams. Foams are a simpler subset of composite materials since they are composed of gas pores contained in a continuous solid matrix. Metallic foams have been used for several decades. Carbon foams are a relatively new class of organic materials that offer significant potential for lightweight structures, for energy absorption and for thermal management [1].

Carbon occurs in many different forms with widely differing thermal properties. Conductivities of approximately $2000 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ are obtained in the plane of the graphene sheets; the conductivity perpendicular to the graphene layers is approximately $6 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. However, carbon foams tend to be more isotropic; the maximum variation in the two directions of highly graphitic foam is typically of a factor of 3. The bulk conductivity for carbon foams ranges from $0.1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ to $200 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$.

Carbon foams are often made by foaming a pitch material. An example of such a foam is shown in Fig. 1. This is a carbon foam that is 90% porous; however, it can have a bulk

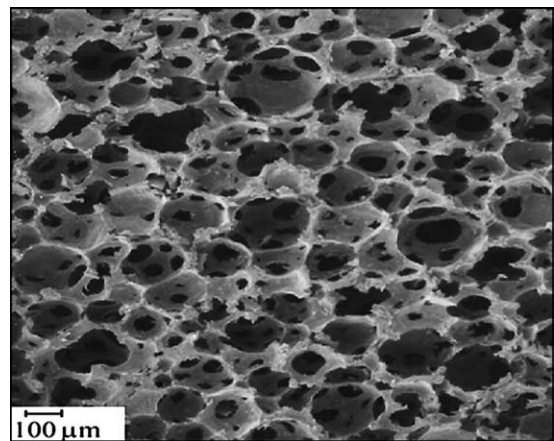


Fig. 1. Micrograph of a graphitic carbon foam.

thermal conductivity exceeding $50 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. The cells are interconnected, and the open cell structure varies from process to process; the pore diameter is approximately 100 microns. Foams of different porosities and pore sizes can be produced by variations of the foaming process.

In the foaming process, a molten pitch precursor is expanded from a high pressure. This leads to the expansion of microscopic gas bubbles within the pitch. Initially the bubbles are in closed pores. As the bubbles expand, the pores become interconnected. The foam is cooled and then

* Corresponding author.

E-mail address: alam@ohio.edu (M.K. Alam).

Nomenclature

a	size of the unit cell	m	n	pore conduction factor	
B	constant determining the temperature field inside a pore			ρ_b	bulk foam density $\text{kg}\cdot\text{m}^{-3}$
C	multiplier of the dipole temperature field perturbation			ρ_s	intrinsic density of the solid $\text{kg}\cdot\text{m}^{-3}$
D	diameter of the pore	m	P	porosity of the porous material, $= \frac{V_{\text{void}}}{V_{\text{total}}}$ %
K	thermal conductivity	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	R	relative density, $= \frac{\rho_b}{\rho_s}$	
K_b	bulk thermal conductivity	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	T	temperature K
K_s	solid (intrinsic) thermal conductivity	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	V_{void}	volume occupied by pores m^3
K_e	effective thermal conductivity of the porous medium	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	V_{total}	total volume of foam m^3
K_p	thermal conductivity of pore material	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	q_z	specific heat flux in z direction (along the porous slab) $\text{W}\cdot\text{m}^{-2}$
				ΔT	temperature difference between two points on the slab K

subjected to heat treatment to stabilize and carbonize the product. This produces foams that have thermal conductivity of about $1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. The foam can be graphitized by a final heat treatment to produce bulk thermal conductivity exceeding $100 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$.

High porosity (above 90% porous) foam that is made of poorly conducting solid conducts heat primarily by conduction in the gas pores; radiation and convection in the pores can also be significant [2]. However, if the solid has good thermal conductivity ($\gg 1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$), the transport through the solid dominates, such that the bulk thermal conductivity tends to exceed $1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$.

In this analysis, only thermal conduction in the solid carbon phase will be considered. At lower temperatures, the gas phase does not contribute significantly to the transport properties in foams that have small pores and moderate (or high) conductivity. This is because the gas conduction is poor and convection and radiation are not significant. Therefore, the thermal transport process in the bulk is dominated by the intrinsic thermal conductivity of the solid. The shape of pores and the total amount of porosity also influence the thermal transport. Some authors have used the rule-of-mixtures to determine thermal conductivity of a composite material even though it is valid only for extensive thermodynamic properties [3]. This rule considers the composite properties as volume-weighted averages of the component properties; and this gives the upper limit for the conductivity of the foam. However, the heat flow path in foams is very tortuous; this produces additional resistance to the conduction process; therefore the thermal conductivity obtained by rule-of-mixtures over-estimates the thermal conductivity. The general practice is to determine the bulk thermal conductivity experimentally by finding the ratio of heat flux to the applied temperature gradient in the foam.

Analytical predictions of thermal properties of porous materials have been presented by several authors [4,5]. A full

theoretical analysis is possible only for low porosity materials. Very high porosity (e.g., low density foams) materials are difficult to model analytically. The typical analysis for such materials tends to be semi-empirical models in which conduction, convection and radiation contributions are added [2,6]. A comprehensive theoretical model was attempted by Bauer to predict the thermal conductivity through the porous media [5]. In this model, analytical expressions were presented for pore distributions of any concentration, randomly oriented pores of arbitrary shape, and radiant heat transfer within the pores. However, in this model, the effect of increasing porosity and pore geometry was lumped into a semi-empirical pore shape factor (a conduction parameter) that must be known a priori or determined experimentally. This pore shape factor is known accurately only for low porosity media with spherical pores [7].

In this study, the focus is on developing a finite element model (FEM) of conduction transport in open and closed cell carbon foams with different levels of porosity. The effect of convection and radiation within the pores will not be considered. The thermal conductivity through the bulk is found by finding the flux through the foam when it is subjected to a thermal gradient. The results are then compared with the analytical approach developed by Bauer and the “conduction parameter” is determined numerically for different porosity levels [5]. The relation between the bulk thermal conductivity and the intrinsic conductivity of the solid is then evaluated in terms of this conduction parameter.

The foam will be modeled by considering a homogeneous dispersion of spherical voids in a solid matrix. A microscopic scale finite element grid is generated within the solid material of the foam. The microstructure of the solid in the foam will be considered to be isotropic in this model. In highly graphitic foams the microstructure is not isotropic because the graphene planes tend to align with the cell walls [1]. In these foams the microstructure is anisotropic in the

same manner that graphite is anisotropic. It should be noted that this approximation restricts the validity of the model to near isotropic foams. Examples of such foams are reticulated vitreous carbon (RVC) foams, glassy carbon foams, and foams that are not highly graphitic.

2. Theory

Several models have been proposed to predict the thermal conductivity of porous materials, including foams. Thermal conductivity in foams was first studied primarily for insulating foams and several studies have discussed the thermal conductivity of insulating, high porosity foams [2,6].

In the present study, the effective thermal conductivity of the open and closed cell foams is determined by using the finite element method. The results are compared with the analytical models. For the analysis, we will use the relative density R as a parameter. It is assumed that the mass of the voids in the foam is negligible. The relative density is defined as:

$$R = \frac{\rho_b}{\rho_s} = 1 - \frac{P}{100} \quad (1)$$

where ρ_b is the bulk foam density, ρ_s is the intrinsic density of the solid in the foam, and P is the porosity (%) or the void content of the foam, defined as:

$$P = 100 \frac{V_{\text{void}}}{V_{\text{total}}} \quad (2)$$

where

V_{void} —volume occupied by pores [m^3];
 V_{total} —total volume of foam [m^3].

From thermodynamic consideration, the value of thermal conductivity of a foam with non-conducting pores has a limiting value given by:

$$K_b \leq K_s \left(\frac{\rho_b}{\rho_s} \right) \quad (3)$$

The maximum value is obtained when the porous solid presents the minimum resistance to heat flow; this represents the rule of mixtures. In practice, the flow path is tortuous, and the true value is always less than the maximum predicted by Eq. (1). Several authors have used a conduction parameter termed “inefficiency factor” or “pore shape factor” to modify the equation. A factor of 2/3 was used by Hillyard and Cunningham to correct for the flow path [8].

A more rigorous approach was adopted by Bauer who considered the perturbation of a continuous medium by the presence of pores [5]. This approach will be compared with the results of this study. The analytical solution is obtained from the perturbation of a uniform temperature gradient in the z direction in a uniform medium due to presence of a spherical pore. By solving the temperature profile, one obtains the following differential equation for the change in

the bulk thermal conductivity K_b in the porous medium as a function of porosity in the medium:

$$\frac{dK_b}{K_b} = - \frac{1 - K_p/K_b}{n + (1 - n)K_p/K_b} \frac{dV}{V} \quad (4)$$

In the above equation, K_p is the conductivity of the pores, K_b is the thermal conductivity of the bulk material that changes as the porosity increases due to increase in the total pore volume V . The new constant n is a “conduction parameter” sometimes called “pore shape factor.” This factor has a maximum value of unity. The rule of mixtures described above is represented by $n = 1$.

Integrating the above equation from $V = 0$ to the final porosity value, one obtains the following equation:

$$\frac{K_b - K_p}{K_s - K_p} \left(\frac{K_s}{K_b} \right)^{1-n} = 1 - (P/100) \quad (5)$$

We will consider the case where the solid conductivity as well as the bulk conductivity is much higher than the pore (gas) conductivity. For this special case where $K_p \ll K_b < K_s$, we obtain the following equation:

$$K_b/K_s = K_e = (1 - P/100)^{1/n} = R^{1/n} \quad (6)$$

In the above equation, K_e is the effective thermal conductivity, defined here as the ratio between the bulk and solid thermal conductivity in the z direction. In the present study, the case represented by Eq. (6) will be investigated; i.e., the conduction through the pores will be neglected and all conduction will be assumed to take place through the solid.

It is important to note that the pore conduction parameter n is generally not known since it changes with pore shape and pore concentration. Therefore, this is a semi-empirical constant. When the porosity is very low, the value of n has been theoretically shown to be 2/3 (i.e., 0.67) for spherical pores [7]. From the study carried out by Bauer, the value of n for closed cell liquid foams with a porosity in the range of 60 to 95% was estimated from experimental results to be $n = 0.77$ [5]. The rule of mixtures, given by $n = 1$, gives the upper limit. These three predictions of thermal conductivity will be compared with FEM results in this study.

Several authors have addressed the problem of determining thermal transport in foams. Kuhn et al. determined the thermal conductivity of foam insulation by approximating the foam to be made of dodecahedron cells [9]. The struts and walls were further simplified into a simple cubic model where structural elements were taken either parallel or vertical to the bulk temperature gradient. Analytical techniques such as homogenization can also be used to determine the bulk thermal properties [10]. In this study, the finite element method (FEM) will be used to determine the bulk thermal conductivity. Due to recent enhancements in FEM software, it is now possible to analyze very complex foam geometry with different pore shapes and sizes. The FEM analysis can also be extended to include effect of radiation and convection, as well as fluid flow through the foam.

The thermal conductivity value obtained by using FEM will be compared with the analytical results given by Eq. (6). The purpose of this study is to investigate the value of the pore conduction parameter n for a simple isotropic material with porosities ranging from zero to very high values (95%). The basic pore shape that will be used is a sphere; however, at high porosity level, the pores become interconnected and the pores are no longer true spheres.

3. Finite element method

The finite element method is widely used to solve structural problems; and has now been adapted to the field of heat transfer analysis. To analyze the thermal field in the foam microstructure, we consider the governing differential equation of steady state heat conduction without internal heat generation in the foam. The foam piece is sandwiched between two slabs of non-porous solid as shown in Fig. 2.

The steady-state heat conduction equation applied to the model in Fig. 2 is given by:

$$\nabla \cdot (K \nabla T) = 0 \quad (7)$$

with the boundary conditions:

$$T = T_1 \quad \text{at the lower bottom face of the slab}$$

$$T = T_2 \quad \text{at the top face of the slab and}$$

$$\frac{\partial T}{\partial n} = 0 \quad \text{on all other surfaces}$$

An important step in this numerical model is to reduce computational effort by creating a unit cell of the porous medium. The unit cell that will be used to build the solid model, consists of a cube with 1/8 spherical shape pores at each corner and one sphere in the middle of the cell as shown in Fig. 3. Therefore, the pores in the foam model have a body centered cubic cell arrangement. Several different arrangements are possible, such as face centered cubic, tetragonal cells, etc.; the effect of different arrangements will be addressed in a future study.

To maintain the structural integrity of the model, the size of the cubic cell is restricted to the values given by:

$$a\sqrt{2} \leq D < a\sqrt{3} \quad (8)$$

Because of the symmetry of the geometry as shown in Fig. 2, the FEM model needs to use only a set of cells in the vertical direction. Therefore, the complete model for FEM analysis in this study is constructed by repeating the unit cell (Fig. 3) ten times in the vertical direction as shown in Fig. 4.

The solid model was analyzed by ALGOR FEM software to predict the temperature and heat flux distribution in the porous media. The solid model was first created with a specialized solid modeling software (Solid Edge) and the geometry was exported as an IGES file which was read directly into the finite element editor of ALGOR.

ALGOR provides an automatic mesh generator that allows building surface and solid meshes that are either uniform or concentrated around critical regions. The size of

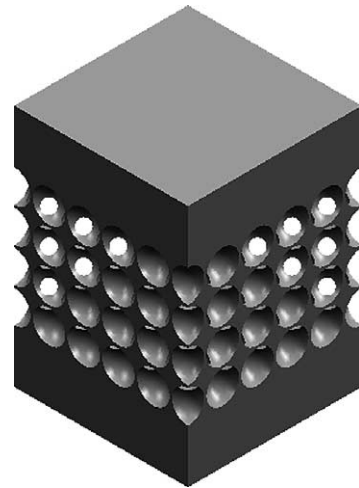


Fig. 2. Foam solid model.

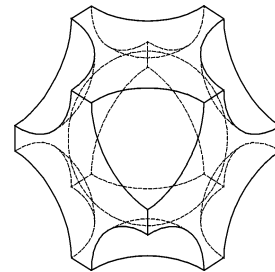


Fig. 3. Unit cell used to model the porous medium.



Fig. 4. Solid model for FEM analysis.

the mesh can be specified either as relative to the dimensions of the model (percentage of the smallest characteristic dimension of the model) or as absolute value (absolute dimension of the edge length).

For the present study, the models were meshed using a quadrilateral surface mesh and the relative size option mesh

provided by ALGOR. The mesh size used for the analysis was between 15% and 25% of the smallest characteristic dimension of the model. The mesh size varied according to the void volume of the model. The higher the void volume, the smaller the mesh size since the solid dimensions become smaller with increased void volume. Using the surface mesh generated, ALGOR builds a solid mesh that consists of eight-noded bricks, tetrahedrons, pyramids and wedges. In order to increase the accuracy of the FEM solution, the mesh was refined around the spherical pores.

After the mesh has been generated, the boundary conditions were applied to the mesh. This involved applying the temperature boundary conditions at the top and the bottom surface. To ensure one-dimensional heat flow along the model in the z -direction, boundary surfaces of the model in both x - and y -directions are given a symmetry (insulated) boundary condition. The other boundary condition imposed was a zero heat flux (since thermal conductivity in the gas phase is much smaller compared to the solid phase) normal to the surface of the spherical pores. As discussed earlier, conduction through the pores was expected to be negligible in this analysis. This assumption can be relaxed in the numerical model for foams where the gas pores provide significant thermal transport.

The finite element solution of Eq. (7) is carried out over the entire domain and the temperature profile in the porous medium is determined. The heat flux in z direction, q_z , was calculated within the software.

Since the heat flux at the top and bottom must be identical to the flux (per unit area of the bulk material) through the porous medium, the bulk thermal conductivity, K_b is then calculated using as follows:

$$K_b = \frac{q_z}{(\Delta T / \Delta z)} \quad (9)$$

where q_z is the heat flux applied at the ends, and $\Delta T / \Delta z$ is the temperature gradient in the foam. The pore size was selected to be 100 microns at 90% porosity, which is representative of the foam shown in Fig. 1. The porosity in the foam is changed by increasing the radius of the void (which reflects the manner in which the foaming process generates the foam); this results in foam models with different degrees of porosity. The effect of changing the pore size is currently under investigation, and is not addressed in this paper. The FEM analysis was conducted over a range of 0% to 95% porosity in the porous region, and the results were compared to analytical solution for a pore shape factor of $n = 0.67$ (spherical pores, low porosity) and $n = 0.77$ (experimental data for closed-cell liquid foams), and $n = 1$ (rule of mixtures).

4. Results

The temperature and heat flux distribution for a porous region of 90% porosity are presented in the Figs. 5 and 6.

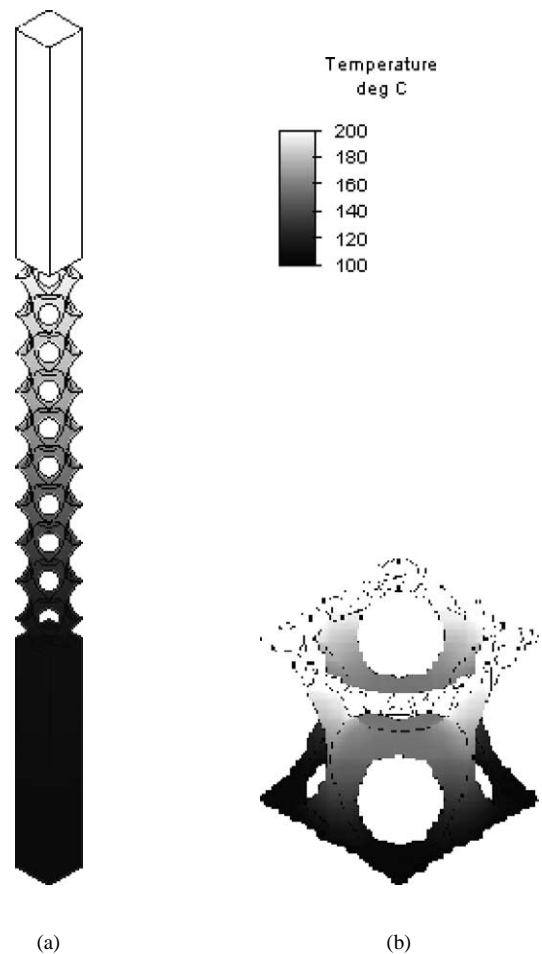


Fig. 5. Temperature distribution in the foam (90% porosity): (a) Full scale model; (b) Unit cell detail.

Fig. 5 shows the temperature distribution results from the finite element model. From Fig. 5 it can be observed that the temperature distribution is mostly one-dimensional in most of the solid phase except near the pores. There is no temperature field shown in the pores since the pores are assumed to be insulated.

Fig. 6 shows the heat flux distribution for the same case. The heat flux varies in the walls of the pores since greater heat flux must occur in the thinner cell walls. However, the heat flux in the two plates (top and bottom) is constant and identical, as is expected.

The results of the finite element analysis as well as the analytical results given by Eq. (6) for different values of n are compared in Fig. 7 as a function of porosity. From Fig. 7 it can be seen that, at the two extremes of 0% and 100% porosity, all solutions converge properly to the limiting values of $K_e = 1$ and $K_e = 0$. The focus of this study is to determine the exponent n for different values of porosity using the numerical analysis. The FEM solution is lower than the rule of mixtures ($n = 1$) throughout the full range of porosities. The analytical curve for $n = 0.67$ matches the FEM solution only at very low porosities (below 10%). This is to be expected, since the theoretical model

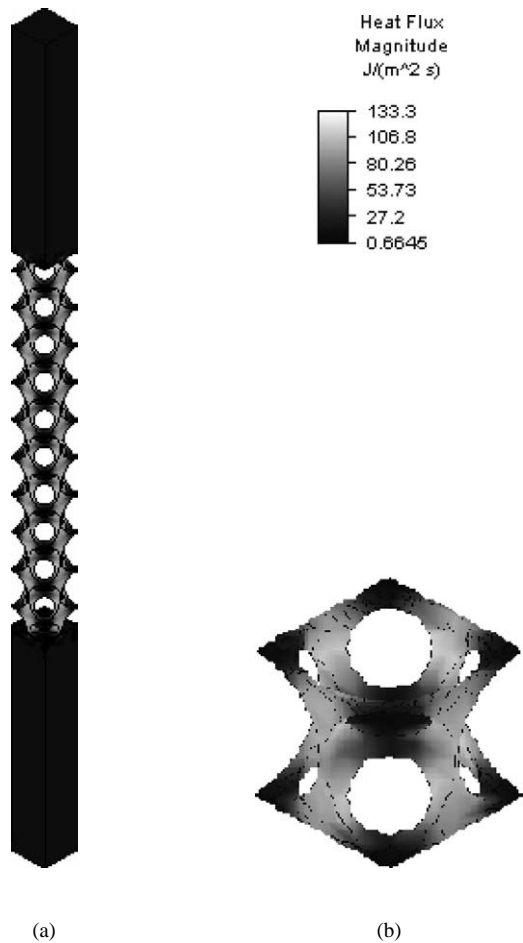


Fig. 6. Heat flux distribution through the foam (90% porosity): (a) Full scale model; (b) Unit cell detail.

that predicts n to be 0.67 is based on the assumption of low porosity. The analytical curve for $n = 0.77$ is closer to the FEM solution for a wide range of porosity; however, it produces a higher value of thermal conductivity in the mid-range of porosities, and a lower value at high porosity. The transition appears to be at the point where the pores become interconnected at 68% porosity. Overall, it is seen that the thermal conductivity cannot be predicted accurately by Eq. (6) with a single value of n for the full range of porosity. The appropriate value of n required to match the FEM solution is seen to be 0.67 at low porosity (below 10%), which increases gradually to a value of 0.854 at 95% porosity.

The effect of changing the number of the unit cells (elemental reference volumes) in the model was studied (Fig. 8). It was determined that models with fewer than ten cells produced more than 1% error in the results. Therefore, the FEM calculations are based on a geometry composed of ten unit cells.

Table 1 shows the difference between effective thermal conductivity calculated using the FEM and semi-empirical solutions for different porosities. The relative error between

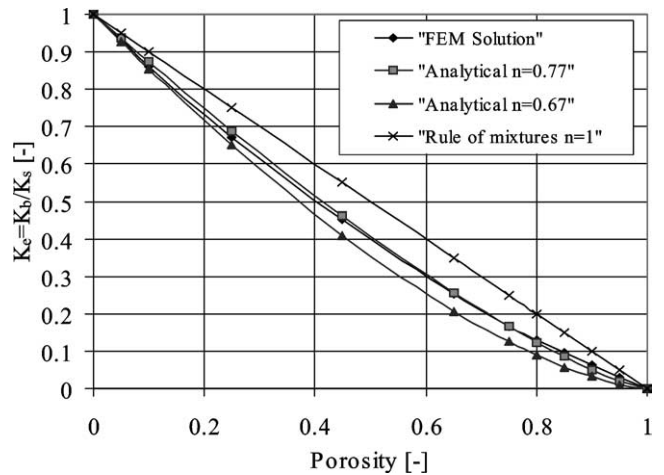


Fig. 7. Variation of effective thermal conductivity with porosity.

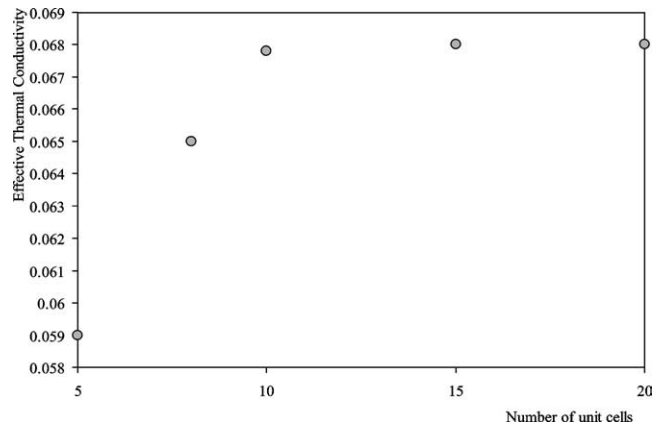


Fig. 8. Variation of effective thermal conductivity with the number of unit cells.

Table 1
Comparison between FEM method and semi-empirical solution

Porosity	Effective thermal conductivity		Relative error [%]
	FEM solution	Semi-empirical $n = 0.77$	
0.25	0.69570	0.6882	0.978
0.45	0.496814	0.4600	7.41
0.85	0.100936	0.0850	15.79
0.95	0.028218	0.0204	27.71

the two solutions is increasing from 1% at low porosity to a maximum value of 28% at high porosity. Since the typical carbon foam is produced with high porosity, the errors are significant for carbon foams.

The value of the parameter n is expected to be different when the pore shape is not spherical, and when the material of the foam is not isotropic. The FEM model developed in this study will be used to model foams that are non-isotropic and non-homogeneous, with different types of pores and pore distributions.

5. Conclusions

A finite element model has been used to determine the thermal conductivity of foams over the full range of porosities. The foam model was constructed by a solid modeling software using spherical pores that became interconnected at high porosities.

The thermal conductivity result was obtained in the form of a non-dimensional effective thermal conductivity. This FEM solution was then used to evaluate the “pore conduction factor” used in semi-empirical/analytical models of thermal conductivity.

The FEM solution matches the theoretical prediction at the low porosity level. But significant difference is observed between the FEM simulation and analytical results for high porosity foams. The results also show that a simple semi-empirical or analytical model with a constant “conduction parameter” cannot accurately predict the thermal conductivity of foams over the full range of porosity. In this study, the value of this parameter increased from the theoretical value of 0.67 at low porosity, to approximately 0.83 at 90% porosity.

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