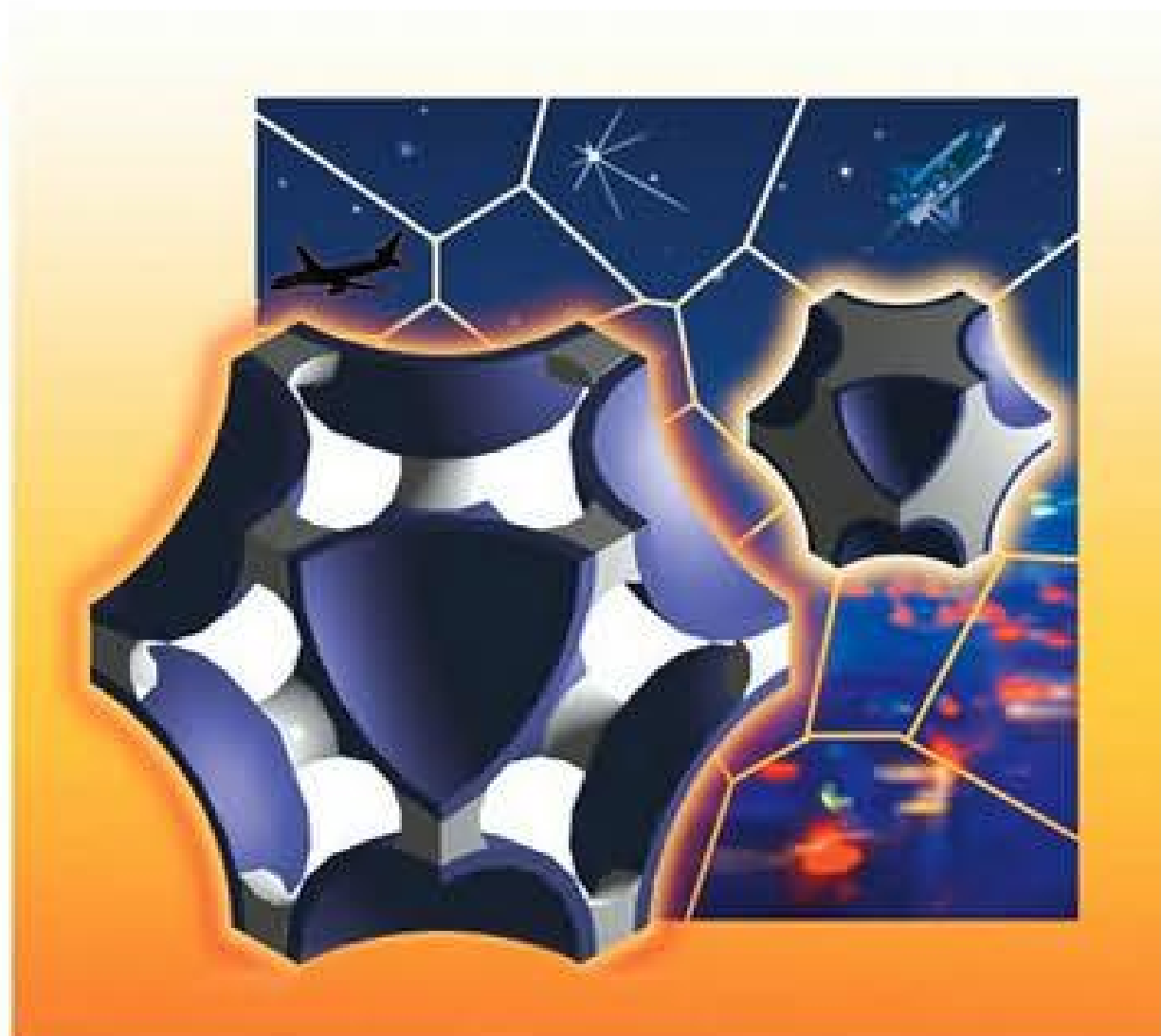


Andreas Öchsner, Graeme E. Murch,
Marcelo J. S. de Lemos (Eds.)

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Cellular and Porous Materials

Thermal Properties Simulation and Prediction



Cellular and Porous Materials

Edited by
Andreas Öchsner, Graeme E. Murch,
and Marcelo J. S. de Lemos

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Preface

Nature frequently uses cellular and porous materials for creating load-carrying and weight-optimized structures. Thanks to their cellular design, natural materials such as wood, cork, bones, and honeycombs fulfill structural as well as functional demands. For a long time, the development of artificial cellular materials has been aimed at utilizing the outstanding properties of biological materials in technical applications. As an example, the geometry of honeycombs was identically converted into aluminum structures which have been used since the 1960s as cores of lightweight sandwich elements in the aviation and space industries. Nowadays, in particular, foams made of polymeric materials are widely used in all fields of technology. For example, Styrofoam[®] and hard polyurethane foams are widely used as packaging materials. Other typical application areas are the fields of heat and sound absorption. During the last few years, techniques for foaming metals and metal alloys and for manufacturing novel metallic cellular structures have been developed. Owing to their specific properties, these cellular materials have considerable potential for applications in the future. The combination of specific mechanical and physical properties distinguishes them from traditional dense metals, and applications with multifunctional requirements are of special interest in the context of such cellular metals. Their high stiffness, in conjunction with a very low specific weight, and their high gas permeability combined with a high thermal conductivity can be mentioned as examples. Cellular materials comprise a wide range of different arrangements and forms of cell structures. Metallic foams are being investigated intensively, and they can be produced with a closed- or open-cell structure. Their main characteristic is their very low density. The most common foams are made of aluminum alloys. Quite a regular arrangement of cells is obtained in structures, e.g. with hollow spheres. A perfect regular structure results from interconnecting networks of straight beams; materials of this type are known as lattice block materials. What all these different cellular materials have in common is that their physical properties are not only determined by their cell wall material but also significantly by their microstructure.

Several textbooks cover the topic of cellular materials in general and give an introduction to the whole range of physical properties and possible applications. The books by L. J. Gibson and M. F. Ashby (Pergamon Press, 1988), M. F. Ashby *et al.*

(Butterworth Heinemann, 2000), and H.-P. Degischer and B. Kriszt (Wiley-VCH, 2002) are recognized as standard works on this topic and give the most comprehensive general overview of cellular and porous materials.

The idea of this book is to cover one of the important physical characteristics, i.e. thermal properties, in detail from different points of view. This book aims to provide readers not only with a good understanding of the fundamentals but also with an awareness of recent advances in properties determination and applications of cellular and porous materials. The book contains 12 chapters written by experts in the relevant fields from academia and from major national laboratories/research institutes. The first part of the book introduces in detail different numerical and analytical methods in order to characterize and predict the effective thermal properties. Each of these chapters focuses on a detailed introduction of the theoretical and/or experimental method(s) which are applied to the characterization of different materials. The first part of the book introduces aspects relevant even for a non-specialist, i.e. to provide information which is normally omitted in the scope of journal publications. Different characterization approaches are presented and applied to different types of cellular and porous materials in order to reveal a spectrum for the investigation of effective thermal properties. The second part of the book addresses various types of applications and specialized topics related to the context of thermal properties of cellular and porous materials.

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January 2008

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1

Interfacial Heat Transport in Highly Permeable Media: A Finite Volume Approach

Marcelo J.S. de Lemos and Marcelo B. Saito

1.1

Introduction

The transport of heat inside highly permeable media has attracted the attention of scientists and engineers due to its many engineering applications. Such applications can be found in solar energy receiver devices, heat exchangers, porous combustors, grain drying equipment, heat sink units, energy recovery systems, etc. In many of these modern engineering systems the use of cellular and metallic porous foams brings the advantages of having large specific heat transfer areas, or the interfacial transport area per unit volume is large when compared with other heat-capturing devices. More realistic modeling of transport processes in such media is then essential for the reliable design and analysis of high-efficiency engineering systems.

Motivated by the wide spectrum of practical engineering applications, macroscopic transport modeling of incompressible flows in porous media has been developed over the last few decades, mostly based on the volume-average methodology for either heat [1] or mass transfer [2,3]. Classic books by Bear (1972) [4], Nield and Bejan (1992) [5] and Ingham and Pop (1998) [6], to mention a few, also document forced convection and related models for heat transport in porous media.

From the point of view of energy transfer between phases, namely the cellular material phase and the working fluid, there are basically two different models commonly found in the literature: (a) a *local thermal equilibrium* model and (b) a *two-energy equation* or *thermal nonequilibrium* model. The first one assumes that the bulk solid temperature does not differ much from the average value of the fluid temperature; thus local thermal equilibrium between the fluid and the solid phase is assumed. This model greatly simplifies theoretical and numerical research but the assumption of local thermal equilibrium between the fluid and the solid is inadequate for a number of practical problems [7–9]. As a result, in recent years more attention has been paid to the local thermal nonequilibrium model, both theoretically and numerically [10,11].

Accordingly, *two-energy equation models* have been investigated by a number of researchers. Kuwahara *et al.* (2001) [12] proposed a numerical procedure to determine macroscopic transport coefficients from a theoretical basis without any empiricism. They used a single unit cell and determined the interfacial heat transfer coefficient for the asymptotic case of infinite conductivity of the solid phase. Nakayama *et al.* (2001) [13] extended the conduction model of Hsu (1999) [14] for treating also convection in porous media. Having established the macroscopic energy equations for both phases, useful exact solutions were obtained for two fundamental heat transfer processes associated with porous media, namely steady conduction in a porous slab with internal heat generation within the solid and also thermally developing flow through a semi-infinite porous medium. Saito and de Lemos (2005) [15] considered the distribution in cell parameters and, after volume-averaging them, the interfacial heat transfer coefficient for laminar flow.

In all of the above, only laminar flow has been considered. When treating turbulent flow in porous media, however, difficulties arise due to the fact that the flow fluctuates with time and a volumetric average is applied [16]. For handling such situations, a new concept called *double decomposition* has been proposed for developing macroscopic models for turbulent transport in porous media [17–22]. This methodology has been extended to nonbuoyant heat transfer [23], buoyant flows [24–30], mass transfer [31] and double diffusion [32]. In addition, a general classification of models has been published [33]. Further, the problem of treating interfaces between a porous medium and a clear region, considering a diffusion-jump condition for laminar [34] and turbulence fields [35–37], has also been investigated under the concept first proposed by several authors [17–22]. Furthermore, Saito and de Lemos (2006) [38] proposed a new correlation for obtaining the interfacial heat transfer coefficient for turbulent flow in a packed bed, which is modeled as an infinite staggered array of square rods. Recently, a book has been published on the subject of turbulence modeling in porous media [39].

Motivated by the foregoing, this chapter focuses on laminar and turbulent flow through a packed bed, which represents an important configuration for efficient heat and mass transfer and suggests the use of equations governing thermal nonequilibrium involving distinct energy balances for both the solid and fluid phases. Hence, the use of such a two-energy equation model requires an extra parameter to be determined, namely the heat transfer coefficient between the fluid and the solid. This chapter reviews recent efforts in proposing correlations for obtaining the interfacial heat transfer coefficient for laminar and turbulent flow in porous material. The medium is here modeled as an infinite array of rods of distinct shapes, over which the range of Reynolds number, based on a characteristic size of the rod, is extended up to 10^7 .

The next sections detail the basic mathematical model, including the mean and turbulent fields for turbulent flows. Although the discussion of turbulent motion in porous media is not presented, the definitions and concepts to calculate the interfacial heat transfer coefficient for macroscopic flows are presented here.

1.2

Governing Equations

1.2.1

Microscopic Transport Equations

Local time-averaged transport equations for incompressible fluid flow in a rigid homogeneous porous medium have already been presented in the literature and their derivation need not be repeated here [24]. The governing equations for the flow and energy for an incompressible fluid are given by

$$\text{Continuity: } \nabla \cdot \mathbf{u} = 0 \quad (1.1)$$

$$\text{Momentum: } \rho \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right] = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (1.2)$$

$$\text{Energy—fluid phase: } (\rho c_p)_f \left\{ \frac{\partial T_f}{\partial t} + \nabla \cdot (\mathbf{u} T_f) \right\} = \nabla \cdot (k_f \nabla T_f) + S_f \quad (1.3)$$

$$\text{Energy—solid phase (porous matrix): } (\rho c_p)_s \frac{\partial T_s}{\partial t} = \nabla \cdot (k_s \nabla T_s) + S_s \quad (1.4)$$

where the subscripts f and s refer to fluid and solid phases, respectively. Here, T is the temperature, k_f is the fluid thermal conductivity, k_s is the solid thermal conductivity, c_p is the specific heat and S is the heat generation term. If there is no heat generation either in the solid or in the fluid, one further has $S_f = S_s = 0$.

For turbulent flows the time-averaged transport equations can be written as

$$\text{Continuity: } \nabla \cdot \bar{\mathbf{u}} = 0 \quad (1.5)$$

$$\text{Momentum: } \rho_f [\nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}})] = -\nabla \bar{p} + \nabla \cdot \left\{ \mu [\nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^T] - \rho \overline{\mathbf{u}'\mathbf{u}'} \right\} \quad (1.6)$$

where the low and high Reynolds $k-\varepsilon$ models as can be used to calculate the Reynolds stresses $\overline{\rho \mathbf{u}'\mathbf{u}'}$ via the eddy viscosity concept, μ_t . Equations for the turbulent kinetic energy per unit mass (TKE) and for its dissipation rate read:

Turbulent kinetic energy per unit mass (TKE):

$$\rho_f [\nabla \cdot (\bar{\mathbf{u}}k)] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] - \rho \overline{\mathbf{u}'\mathbf{u}'} : \nabla \bar{\mathbf{u}} - \rho \varepsilon \quad (1.7)$$

TKE dissipation rate:

$$\rho_f [\nabla \cdot (\bar{\mathbf{u}}\varepsilon)] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \left[c_1 (-\rho \overline{\mathbf{u}'\mathbf{u}'} : \nabla \bar{\mathbf{u}}) - c_2 f_2 \rho \varepsilon \right] \frac{\varepsilon}{k} \quad (1.8)$$

The Reynolds stresses and the eddy viscosity are given by, respectively:

$$-\rho \overline{\mathbf{u}'\mathbf{u}'} = \mu_t \left[\nabla \overline{\mathbf{u}} + (\nabla \overline{\mathbf{u}})^T \right] - \frac{2}{3} \rho k \mathbf{I} \quad (1.9)$$

$$\mu_t = \rho c_\mu f_\mu \frac{k^2}{\varepsilon} \quad (1.10)$$

where ρ is the fluid density, p is the pressure and μ represents the fluid viscosity.

In the above equation set, σ_k , σ_ε , c_1 , c_2 and c_μ are dimensionless constants whereas f_2 and f_μ are damping functions used with the so-called low Re $k - \varepsilon$ turbulence models. The following damping functions are adopted here when computing with the low Re model:

$$f_\mu = \left\{ 1 - \exp \left[-\frac{(v\varepsilon)^{0.25} \gamma}{14\nu} \right] \right\}^2 \left\{ 1 + \frac{5}{(k^2/v\varepsilon)^{0.75}} \exp \left[-\left(\frac{(k^2/v\varepsilon)}{200} \right)^2 \right] \right\} \quad (1.11)$$

$$f_2 = \left\{ 1 - \exp \left[-\frac{(v\varepsilon)^{0.25} \gamma}{3.1\nu} \right] \right\}^2 \left\{ 1 - 0.3 \exp \left[-\left(\frac{(k^2/v\varepsilon)}{6.5} \right)^2 \right] \right\} \quad (1.12)$$

where γ is the coordinate normal to the wall. Other constants are given as $c_\mu = 0.09$, $c_1 = 1.5$, $c_2 = 1.9$, $\sigma_k = 1.4$, $\sigma_\varepsilon = 1.3$, which were taken from Launder and Spalding (1974) [40].

Also, the time-averaged energy equations become

Energy–fluid phase:

$$(\rho c_p)_f [\nabla \cdot (\overline{\mathbf{u}} \overline{T}_f)] = \nabla \cdot (k_f \nabla \overline{T}_f) - (\rho c_p)_f \nabla \cdot (\overline{\mathbf{u}'} \overline{T}_f') \quad (1.13)$$

Energy–solid phase (porous matrix):

$$\nabla \cdot (k_s \nabla \overline{T}_s) + S_s = 0 \quad (1.14)$$

1.2.2

Decomposition of Flow Variables in Space and Time

If time fluctuations of the flow properties are also considered, in addition to spatial deviations, there are two possible methodologies to follow in order to obtain macroscopic equations: (a) application of time-average operator followed by volume-averaging [41–46], or (b) use of volume-averaging before time-averaging is applied [47–49]. However, both sets of macroscopic mass transport equations are equivalent when examined under the recently established double decomposition concept [17–22]. As mentioned above, the double decomposition concept has been published in a number of widely available journal articles [17–24], book chapters [50–53] and a

book [39]. For the sake of completeness, a brief overview is presented here and additional details can be found in the literature cited.

Macroscopic transport equations for turbulent flow in a porous medium are obtained through the simultaneous application of time- and volume-average operators over a generic fluid property φ [16]. Such concepts are mathematically defined as

$$\overline{\varphi} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \varphi \, dt, \quad \text{with} \quad \varphi = \overline{\varphi} + \varphi' \quad (1.15)$$

$$\langle \varphi \rangle^i = \frac{1}{\Delta V_f} \int_{\Delta V_f} \varphi \, dV; \quad \langle \varphi \rangle^v = \phi \langle \varphi \rangle^i; \quad \phi = \frac{\Delta V_f}{\Delta V}, \quad \text{with} \quad \phi = \langle \varphi \rangle^i + {}^i\varphi \quad (1.16)$$

where ΔV_f is the volume of the fluid contained in a representative elementary volume (REV) ΔV and intrinsic average and volume average are represented, respectively, by $\langle \rangle^i$ and $\langle \rangle^v$. Also, the left superscript i represents spatial deviation.

The double decomposition idea introduced and fully described elsewhere [17–22], combines Eqs. (1.15) and (1.16) and can be summarized as

$$\overline{\langle \varphi \rangle^i} = \langle \overline{\varphi} \rangle^i; \quad {}^i\overline{\varphi} = \overline{{}^i\varphi}; \quad \langle \varphi' \rangle^i = \langle \varphi \rangle'^i \quad (1.17)$$

and

$$\left. \begin{array}{l} \varphi' = \langle \varphi' \rangle^i + {}^i\varphi' \\ {}^i\varphi = {}^i\overline{\varphi} + {}^i\varphi' \end{array} \right\} \quad \text{where} \quad {}^i\varphi' = \varphi' - \langle \varphi' \rangle^i = {}^i\varphi - {}^i\overline{\varphi} \quad (1.18)$$

Therefore, the quantity φ can be expressed by either

$$\varphi = \overline{\langle \varphi \rangle^i} + \langle \varphi \rangle'^i + {}^i\overline{\varphi} + {}^i\varphi' \quad (1.19)$$

or

$$\varphi = \langle \overline{\varphi} \rangle^i + {}^i\overline{\varphi} + \langle \varphi' \rangle^i + {}^i\varphi' \quad (1.20)$$

The term ${}^i\varphi'$ can be viewed as either the temporal fluctuation of the spatial deviation or the spatial deviation of the temporal fluctuation of quantity φ [39].

1.2.3

Macroscopic Flow and Energy Equations

When the average operators (1.15) and (1.16) are simultaneously applied over Eqs. (1.1) and (1.2), macroscopic equations for turbulent flow are obtained. Volume integration is performed over a REV [16,54], resulting in

$$\text{Continuity: } \nabla \cdot \overline{\mathbf{u}}_D = 0 \quad (1.21)$$

where $\bar{\mathbf{u}}_D = \phi \langle \bar{\mathbf{u}} \rangle^i$ and $\langle \bar{\mathbf{u}} \rangle^i$ identifies the intrinsic (liquid) average of the time-averaged velocity vector $\bar{\mathbf{u}}$.

$$\begin{aligned} \text{Momentum: } \rho \left[\frac{\partial \bar{\mathbf{u}}_D}{\partial t} + \nabla \cdot \left(\frac{\bar{\mathbf{u}}_D \bar{\mathbf{u}}_D}{\phi} \right) \right] &= -\nabla(\phi \langle \bar{p} \rangle^i) + \mu \nabla^2 \bar{\mathbf{u}}_D \\ &- \nabla \cdot (\rho \phi \langle \bar{\mathbf{u}}' \bar{\mathbf{u}}' \rangle^i) - \left[\frac{\mu \phi}{K} \bar{\mathbf{u}}_D + \frac{c_F \phi \rho |\bar{\mathbf{u}}_D| \bar{\mathbf{u}}_D}{\sqrt{K}} \right] \end{aligned} \quad (1.22)$$

where the last two terms in Eq. (1.22) represent the Darcy and Forchheimer contributions [55]. Parameter K is the porous medium permeability, c_F is the form drag or Forchheimer coefficient, $\langle \bar{p} \rangle^i$ is the intrinsic average pressure of the fluid and ϕ is the porosity of the porous medium.

The macroscopic Reynolds stress, $-\rho \phi \langle \bar{\mathbf{u}}' \bar{\mathbf{u}}' \rangle^i$, appearing in Eq. (1.22) is given as

$$-\rho \phi \langle \bar{\mathbf{u}}' \bar{\mathbf{u}}' \rangle^i = \mu_{t_b} 2 \langle \bar{\mathbf{D}} \rangle^v - \frac{2}{3} \phi \rho \langle k \rangle^i \mathbf{I} \quad (1.23)$$

where

$$\langle \bar{\mathbf{D}} \rangle^v = \frac{1}{2} \left[\nabla(\phi \langle \bar{\mathbf{u}} \rangle^i) + [\nabla(\phi \langle \bar{\mathbf{u}} \rangle^i)]^T \right] \quad (1.24)$$

is the macroscopic deformation tensor, $\langle k \rangle^i = \langle \bar{\mathbf{u}}' \cdot \bar{\mathbf{u}}' \rangle^i / 2$ is the intrinsic turbulent kinetic energy and μ_{t_b} is the turbulent viscosity, which is modeled in Ref. [33] similarly to the case of clear flow in the form

$$\mu_{t_b} = \rho c_\mu \frac{\langle k \rangle^i{}^2}{\langle \varepsilon \rangle^i} \quad (1.25)$$

The intrinsic turbulent kinetic energy per unit mass and its dissipation rate are governed by the following equations:

$$\begin{aligned} \rho \left[\frac{\partial}{\partial t} (\phi \langle k \rangle^i) + \nabla \cdot (\bar{\mathbf{u}}_D \langle k \rangle^i) \right] &= \nabla \cdot \left[\left(\mu + \frac{\mu_{t_b}}{\sigma_k} \right) \nabla(\phi \langle k \rangle^i) \right] - \rho \langle \bar{\mathbf{u}}' \bar{\mathbf{u}}' \rangle^i : \nabla \bar{\mathbf{u}}_D \\ &+ c_k \rho \frac{\phi \langle k \rangle^i |\bar{\mathbf{u}}_D|}{\sqrt{K}} - \rho \phi \langle \varepsilon \rangle^i \end{aligned} \quad (1.26)$$

$$\begin{aligned} \rho \left[\frac{\partial}{\partial t} (\phi \langle \varepsilon \rangle^i) + \nabla \cdot (\bar{\mathbf{u}}_D \langle \varepsilon \rangle^i) \right] &= \nabla \cdot \left[\left(\mu + \frac{\mu_{t_b}}{\sigma_\varepsilon} \right) \nabla(\phi \langle \varepsilon \rangle^i) \right] \\ &+ c_1 (-\rho \langle \bar{\mathbf{u}}' \bar{\mathbf{u}}' \rangle^i : \nabla \bar{\mathbf{u}}_D) \frac{\langle \varepsilon \rangle^i}{\langle k \rangle^i} + c_2 c_k \rho \frac{\phi \langle \varepsilon \rangle^i |\bar{\mathbf{u}}_D|}{\sqrt{K}} \\ &- c_2 \rho \phi \frac{\langle \varepsilon \rangle^i{}^2}{\langle k \rangle^i} \end{aligned} \quad (1.27)$$

where c_k , c_1 , c_2 and c_μ are nondimensional constants. The second terms on the left-hand side of Eqs. (1.26) and (1.27) represent the generation rate of $\langle k \rangle^i$ and $\langle \varepsilon \rangle^i$, respectively, due to the mean gradient of $\bar{\mathbf{u}}_D$. The third terms in both equations are related to the generation rates due to the action of the porous matrix [18].

Similarly, macroscopic energy equations are obtained for both fluid and solid phases by applying time and volume average operators to Eqs. (1.3) and (1.4). As in the flow case, volume integration is performed over a REV, resulting in

$$\begin{aligned}
 & (\rho c_p)_f \frac{\partial \phi \langle \bar{T}_f \rangle^i}{\partial t} + (\rho c_p)_f \left[\nabla \cdot \left\{ \phi \left(\langle \bar{\mathbf{u}} \rangle^i \langle \bar{T}_f \rangle^i + \langle {}^i \bar{\mathbf{u}}^i \bar{T}_f \rangle^i + \langle \bar{\mathbf{u}}' T_f' \rangle^i \right) \right\} \right] \\
 & = \nabla \cdot \left[k_f \nabla (\phi \langle \bar{T}_f \rangle^i) + \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_f \bar{T}_f dA \right] + \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i \cdot k_f \nabla \bar{T}_f dA \quad (1.28)
 \end{aligned}$$

$$\begin{aligned}
 & (\rho c_p)_s \left\{ \frac{\partial (1 - \phi) \langle \bar{T}_s \rangle^i}{\partial t} \right\} = \nabla \cdot \left\{ k_s \nabla \left[(1 - \phi) \langle \bar{T}_s \rangle^i \right] - \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_s \bar{T}_s dA \right\} \\
 & \quad - \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i \cdot k_s \nabla \bar{T}_s dA \quad (1.29)
 \end{aligned}$$

where $\langle \bar{T}_s \rangle^i$ and $\langle \bar{T}_f \rangle^i$ denote the intrinsic average temperature of solid and fluid phases, respectively, A_i is the interfacial area within the REV and $\mathbf{n}_i$ is the unit vector normal to the fluid–solid interface, pointing from the fluid towards the solid phase. Equations (1.28) and (1.29) are the macroscopic energy equations for the fluid and the porous matrix (solid), respectively.

Further, using the *double decomposition concept* given by Eqs. (1.17)–(1.20), Rocamora and de Lemos (2000) [23] have shown that the fourth term on the left-hand side of Eq. (1.28) can be expressed as

$$\overline{\langle \mathbf{u}' T_f' \rangle^i} = \overline{\langle (\langle \mathbf{u}' \rangle^i + {}^i \mathbf{u}') (\langle T_f' \rangle^i + {}^i T_f') \rangle^i} = \overline{\langle \mathbf{u}' \rangle^i \langle T_f' \rangle^i} + \overline{\langle {}^i \mathbf{u}'^i T_f' \rangle^i} \quad (1.30)$$

Therefore, in view of Eq. (1.30), Eq. (1.28) can be rewritten as

$$\begin{aligned}
 & (\rho c_p)_f \left[\frac{\partial \phi \langle \bar{T}_f \rangle^i}{\partial t} + \nabla \cdot \left\{ \phi \left(\langle \bar{\mathbf{u}} \rangle^i \langle \bar{T}_f \rangle^i + \langle {}^i \bar{\mathbf{u}}^i \bar{T}_f \rangle^i + \overline{\langle \mathbf{u}' \rangle^i \langle T_f' \rangle^i} + \overline{\langle {}^i \mathbf{u}'^i T_f' \rangle^i} \right) \right\} \right] \\
 & = \nabla \cdot \left[k_f \nabla (\phi \langle \bar{T}_f \rangle^i) + \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_f \bar{T}_f dA \right] + \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i \cdot k_f \nabla \bar{T}_f dA \quad (1.31)
 \end{aligned}$$

The two-energy equation model, considering a heat transfer coefficient between the fluid and solid phases, is then based on the following equations

$$\begin{aligned}
 (\rho c_p)_f \left[\frac{\partial \phi \langle \overline{T_f} \rangle^i}{\partial t} + \nabla \cdot \left\{ \phi \left(\underbrace{\langle \overline{\mathbf{u}} \rangle^i \langle \overline{T_f} \rangle^i}_{\text{I}} + \underbrace{\langle \overline{\mathbf{u}^i T_f} \rangle^i}_{\text{II}} + \underbrace{\langle \overline{\mathbf{u}'}^i \langle \overline{T_f'} \rangle^i}_{\text{III}} + \underbrace{\langle \overline{\mathbf{u}^i T_f'} \rangle^i}_{\text{IV}} \right) \right\} \right] \\
 = \nabla \cdot \left[k_f \nabla (\phi \langle \overline{T_f} \rangle^i) + \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_f \overline{T_f} dA \right] + h_i a_i (\langle \overline{T_s} \rangle^i - \langle \overline{T_f} \rangle^i) \quad (1.32)
 \end{aligned}$$

$$\begin{aligned}
 (\rho c_p)_s \left\{ \frac{\partial (1 - \phi) \langle \overline{T_s} \rangle^i}{\partial t} \right\} = \nabla \cdot \left\{ k_s \nabla [(1 - \phi) \langle \overline{T_s} \rangle^i] - \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_s \overline{T_s} dA \right\} \\
 + h_i a_i (\langle \overline{T_f} \rangle^i - \langle \overline{T_s} \rangle^i) \quad (1.33)
 \end{aligned}$$

where h_i and $a_i = A_i/\Delta V$ are the interfacial convective heat transfer coefficient and surface area per unit volume, respectively. The terms describing the convective transport in Eq. (1.32) have the following physical significance (see Rocamora and de Lemos (2000) [23] for details): I, macroscopic convective transport; II, thermal dispersion associated with deviations of time-averaged local velocity and temperature (note that this term also appears when analyzing laminar convection in porous media); III, turbulent heat flux due to the fluctuating components of macroscopic velocity and temperature; and IV, turbulent thermal dispersion in a porous medium due to both time fluctuations and spatial deviations of both microscopic velocity and temperature.

1.2.4

Macroscopic Two-Energy Equation Modeling

In order to apply Eqs. (1.32) and (1.33) to obtain the temperature fields for turbulent flow in porous media, unknown terms in Eq. (1.32) have to be modeled in some way as a function of the intrinsically averaged temperatures of solid and fluid phases, $\langle \overline{T_s} \rangle^i$ and $\langle \overline{T_f} \rangle^i$, respectively. To accomplish this, a gradient-type diffusion model is used for all unknown terms, i.e. thermal dispersion due to spatial deviations, turbulent heat flux due to temporal fluctuations and turbulent thermal dispersion due to both temporal fluctuations and spatial deviations. Also needed is a model for local conduction. Using these gradient-type diffusion models, we can write

$$\text{Thermal dispersion: } -(\rho c_p)_f (\phi \langle \overline{\mathbf{u}^i T_f} \rangle^i) = \mathbf{K}_{\text{disp}} \cdot \nabla \langle \overline{T_f} \rangle^i \quad (1.34)$$

$$\text{Turbulent heat flux: } -(\rho c_p)_f (\phi \langle \overline{\mathbf{u}'}^i \langle \overline{T_f'} \rangle^i \rangle) = \mathbf{K}_t \cdot \nabla \langle \overline{T_f} \rangle^i \quad (1.35)$$

$$\text{Turbulent thermal dispersion: } -(\rho c_p)_f (\phi \langle \overline{\mathbf{u}^i T_f'} \rangle^i) = \mathbf{K}_{\text{disp,t}} \cdot \nabla \langle \overline{T_f} \rangle^i \quad (1.36)$$

$$\text{Local conduction: } \begin{cases} \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_f \overline{T_f} dA = \mathbf{K}_{f,s} \cdot \nabla \langle \overline{T_s} \rangle^i \\ \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i k_s \overline{T_s} dA = \mathbf{K}_{s,f} \cdot \nabla \langle \overline{T_f} \rangle^i \end{cases} \quad (1.37)$$

For the above expressions, Eqs. (1.32) and (1.33) can be written as

$$\{(\rho c_p)_f \phi\} \frac{\partial \langle \overline{T} \rangle^i}{\partial t} + (\rho c_p)_f \nabla \cdot (\mathbf{u}_D \langle \overline{T_f} \rangle^i) = \nabla \cdot \{ \mathbf{K}_{\text{eff},f} \cdot \nabla \langle \overline{T_f} \rangle^i \} + h_i a_i (\langle \overline{T_s} \rangle^i - \langle \overline{T_f} \rangle^i) \quad (1.38)$$

$$\{(1-\phi)(\rho c_p)_s\} \frac{\partial \langle \overline{T} \rangle^i}{\partial t} = \nabla \cdot \{ \mathbf{K}_{\text{eff},s} \cdot \nabla \langle \overline{T_s} \rangle^i \} + h_i a_i (\langle \overline{T_f} \rangle^i - \langle \overline{T_s} \rangle^i) \quad (1.39)$$

where $\mathbf{K}_{\text{eff},f}$ and $\mathbf{K}_{\text{eff},s}$ are the effective conductivity tensors for the fluid and solid phases, respectively, given by

$$\mathbf{K}_{\text{eff},f} = [\phi k_f] \mathbf{I} + \mathbf{K}_{f,s} + \mathbf{K}_{\text{disp}} + \mathbf{K}_t \quad (1.40)$$

$$\mathbf{K}_{\text{eff},s} = [(1-\phi)k_s] \mathbf{I} + \mathbf{K}_{s,f} \quad (1.41)$$

and $\mathbf{I}$ is the unit tensor.

Further, in order to be able to apply Eq. (1.38), it is necessary to determine the components of the conductivity tensor in Eq. (1.40), i.e. $\mathbf{K}_{f,s}$, $\mathbf{K}_{\text{disp}}$, $\mathbf{K}_t$ and $\mathbf{K}_{\text{disp},t}$. Following Kuwahara and Nakayama (1996) [42] and Quintard *et al.* (1997) [10], this can be accomplished for the thermal dispersion and local conduction tensors, $\mathbf{K}_{\text{disp}}$ and $\mathbf{K}_{f,s}$, by making use of a unit cell subjected to periodic boundary conditions for the flow together with an imposed linear temperature gradient on the porous medium. The dispersion and conduction tensors are then obtained directly from the distributed results within the unit cell by making use of Eqs. (1.34) and (1.37). In addition, the following correlations by Nakayama and Kuwahara (1999) [46] for the thermal dispersion tensor, which are valid for $Pe_D \geq 10$, can be used:

$$\frac{(K_{\text{disp}})_{xx}}{k_f} = 2.1 \frac{Pe_D}{(1-\phi)^{0.1}} \quad \text{for longitudinal dispersion} \quad (1.42)$$

$$\frac{(K_{\text{disp}})_{yy}}{k_f} = 0.052(1-\phi)^{0.5} Pe_D \quad \text{for transverse dispersion} \quad (1.43)$$

where $(K_{\text{disp}})_{xx}$ and $(K_{\text{disp}})_{yy}$ are the longitudinal and transverse components of $\mathbf{K}_{\text{disp}}$, respectively.

The turbulent heat flux and turbulent thermal dispersion components of $\mathbf{K}_{\text{eff},f}$, namely $\mathbf{K}_t$ and $\mathbf{K}_{\text{disp},t}$, respectively, are not determined from a distributed calculation. Instead, they are modeled through the classical eddy diffusivity concept,

similar to Nakayama and Kuwahara (1999) [46]. It should be noticed that these two terms arise only if the flow is turbulent within the void space, whereas the thermal dispersion term, $\mathbf{K}_{\text{disp}}$, exists for both laminar and turbulent flow regimes. Starting out from the time-averaged local energy equation coupled with the standard modeling of the turbulent heat flux through the eddy diffusivity concept, ν_t , one can write

$$-(\rho c_p)_f \overline{\mathbf{u}' T_f'} = (\rho c_p)_f \frac{\nu_t}{\sigma_t} \nabla \overline{T_f} \quad (1.44)$$

where σ_t is the turbulent Prandtl number, which is taken here as a constant.

Applying the volume average to the resulting equation, one obtains the macroscopic version of the turbulent heat flux, given by

$$-(\rho c_p)_f \phi \langle \overline{\mathbf{u}' T_f'} \rangle^i = (\rho c_p)_f \frac{\nu_{t\phi}}{\sigma_t} \nabla \langle \overline{T_f} \rangle^i \quad (1.45)$$

where we have adopted the symbol $\nu_{t\phi}$ to express the macroscopic eddy diffusivity. Now, adding up Eqs. (1.35) and (1.36) in light of Eq. (1.30) one has

$$-(\rho c_p)_f (\phi [\langle \overline{\mathbf{u}'} \rangle^i \langle \overline{T_f'} \rangle^i + \langle \overline{\mathbf{u}'^i T_f'} \rangle^i]) = -(\rho c_p)_f \langle \overline{\mathbf{u}' T_f'} \rangle^i = (\mathbf{K}_t + \mathbf{K}_{\text{disp},t}) \cdot \nabla \langle \overline{T_f} \rangle^i \quad (1.46)$$

According to Eqs. (1.45) and (1.46), the overall turbulent heat transport is the sum of the turbulent heat flux and the turbulent thermal dispersion mechanisms, as proposed by Rocamora and de Lemos (2000) [23]. As suggested by Eq. (1.45), both mechanisms are modeled together, giving for $\mathbf{K}_t$ and $\mathbf{K}_{\text{disp},t}$ the expression

$$\mathbf{K}_t + \mathbf{K}_{\text{disp},t} = \phi (\rho c_p)_f \frac{\nu_{t\phi}}{\sigma_t} \mathbf{I} \quad (1.47)$$

Details of interfacial convective heat transfer coefficient are presented in the next section.

1.2.5

Interfacial Heat Transfer Coefficient

In Eqs. (1.32) and (1.33) the heat transferred between the two phases was modeled by means of a film coefficient h_i such that

$$h_i a_i (\langle \overline{T_s} \rangle^i - \langle \overline{T_f} \rangle^i) = \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i \cdot k_f \nabla \overline{T_f} dA = \frac{1}{\Delta V} \int_{A_i} \mathbf{n}_i \cdot k_s \nabla \overline{T_s} dA \quad (1.48)$$

where a_i , as mentioned, is the interfacial area per unit volume. In foam-like or cellular media, the high values of a_i make them attractive for transferring thermal energy via conduction through the solid followed by convection to a fluid stream.

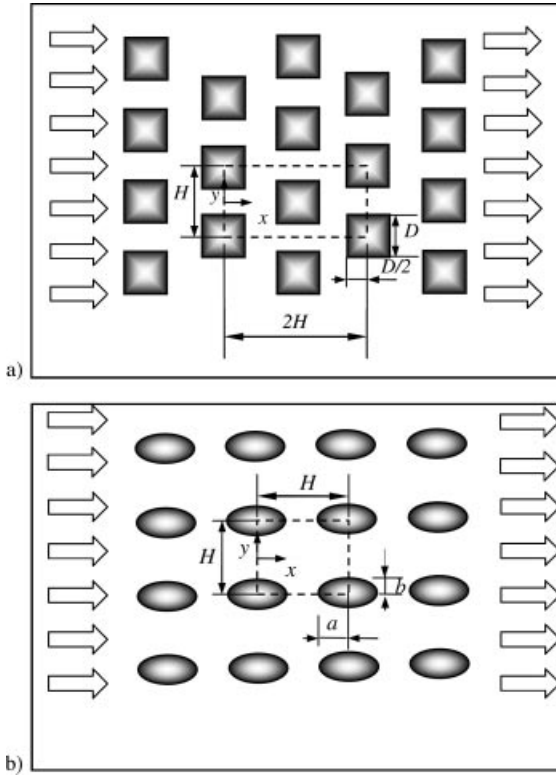


Figure 1.1 Porous media models and coordinate systems: (a) triangular (*staggered*) array of square rods; (b) square (*inline*) array of elliptic rods.

For obtaining macroscopic transport properties, highly permeable media can be modeled as an infinite array of rods, which, in turn, can be analogous to flow across a bundle of tubes. Accordingly, two tube arrangements are generally found in the literature, i.e. the tube rows in a bundle are either inline, with rod centers forming a *square* or a rectangle, or else they are staggered, where a *triangular* shape is obtained when connecting the tube centerlines. In this chapter, the two forms of arrays, namely **square** (*inline*) and **triangular** (*staggered*) layouts are used in order to model flow and heat transfer in highly porous media (see Figure 1.1).

For the staggered configuration of tube banks, Zhukauskas (1972) [56] has proposed a correlation of the form

$$\frac{h_i D}{k_f} = 0.022 Re_D^{0.84} Pr^{0.36} \quad \text{for } 2 \times 10^5 < Re_D < 2 \times 10^6 \quad (1.49)$$

where the values 0.022 and 0.84 are for tubes in cross flow.

Wakao *et al.* (1979) [57] obtained a heuristic correlation for a closely packed bed of particle diameter D and compared their results with experimental data. This correlation for the interfacial heat transfer coefficient is given by

$$\frac{h_i D}{k_f} = 2 + 1.1 Re_D^{0.6} Pr^{1/3} \quad (1.50)$$

For numerically determining h_i , Kuwahara *et al.* (2001) [12] modeled a porous medium by considering it as an infinite number of solid square rods of size D , arranged in a regular triangular pattern (see Figure 1.1). They numerically solved the governing equations in the void region, exploiting to advantage the fact that for an infinite and geometrically ordered medium a repetitive cell can be identified. Periodic boundary conditions were then applied for obtaining the temperature distribution under fully developed flow conditions. A numerical correlation for the interfacial convective heat transfer coefficient was proposed by Kuwahara *et al.* (2001) [12] for laminar flow as

$$\frac{h_i D}{k_f} = \left(1 + \frac{4(1 - \phi)}{\phi}\right) + \frac{1}{2}(1 - \phi)^{1/2} Re_D Pr^{1/3}, \quad \text{valid for } 0.2 < \phi < 0.9 \quad (1.51)$$

Equation (1.51) is based on porosity dependency and is valid for packed beds of particle diameter D . Saito and de Lemos (2005) [15] obtained the interfacial heat transfer coefficient for laminar flows through an infinite square rod using the same methodology as Kuwahara *et al.* (2001) [12].

1.3

Numerical Determination of h_i

1.3.1

Physical Model

Measuring flow and heat transfer characteristics within the void space in foam-like media is a challenging task. However, macroscopic behavior of permeable materials can be obtained by integrating distributed parameters calculated at pore scale. In order to follow such methodology, scientists and engineers have made use of physical models that consider a well-ordered porous medium, which is composed by regularly arranged obstacles instead of randomly distributed solid particles. Assuming further that such medium is of a large size, a repetitive or unit cell can be identified, over which the balance equations are then numerically solved.

Following this path, Kuwahara *et al.* (2001) [12] and Nakayama *et al.* (2001) [13] modeled a porous medium in terms of square obstacles displaced in a regular staggered pattern. They numerically solved the set of local governing equations in a unit or repetitive cell of that arrangement. By volume averaging the distributed

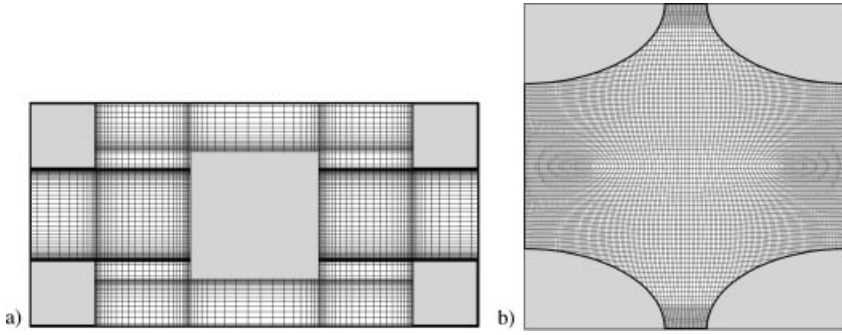


Figure 1.2 Periodic cells and computational grids: (a) triangular (*staggered*) array of square rods; (b) square (*aligned*) array of elliptic rods.

parameters, they got useful information used in calculating the interfacial heat transfer coefficient h_i . Such coefficient, as seen above, is necessary to close the mathematical model when two energy equations, one for the solid and one for the saturating fluid, are solved.

Motivated by the foregoing, this work also applies the methodology of computing first distributed flow parameters in a repetitive cell followed by integration of local values. The periodic cell of volume ΔV used in this work is schematically shown in Figure 1.1. It has dimensions $2H \times H$ for square rods (Figure 1.1a) and $H \times H$ for elliptic obstacles (Figure 1.1b). Computations within those cells were carried out using a nonuniform grid as presented in Figure 1.2. The Reynolds number $Re_D = \rho \bar{u}_D D / \mu$ was varied from 10^4 to 10^7 .

The numerical method utilized to discretize the flow and energy equations in the unit cell was the finite control volume approach. The SIMPLE method of Patankar [58] was used for handling the pressure–velocity coupling. Convergence was monitored in terms of the normalized residue for all variables. The maximum residue allowed before convergence was 10^{-9} , being the variables normalized by appropriate reference values.

For fully developed flow in the cells of Figure 1.1, the velocity at exit ($x/H = 2$ for square rods and $x/H = 1$ for elliptic rods) must be identical to that at the inlet ($x/H = 0$). Temperature profiles, however, are only identical at both cell exit and inlet if presented in terms of an appropriate nondimensional variable. The situation is analogous to the case of forced convection in a channel with isothermal walls. Due to the periodicity of the flow, a single structural unit, as indicated in Figure 1.1, may be taken as a calculation domain. Turbulent flow is modeled by means of Eqs. (1.25), (1.26) and (1.27). Boundary conditions are given by the following.

(a) On the solid walls (laminar or low Re model):

$$\bar{u} = 0, k = 0, \varepsilon = \nu \frac{\partial^2 k}{\partial y^2}, \bar{T} = \bar{T}_w \quad (1.52)$$

(b) On the solid walls (high Re model):

$$\frac{\bar{u}}{u_\tau} = \frac{1}{\kappa} \ln(\gamma^+ E), \quad k = k_w = \frac{u_\tau^2}{c_\mu^{1/2}}, \quad \varepsilon = \frac{c_\mu^{3/4} k_w^{3/2}}{\kappa \gamma_w}, \quad q_w = \frac{(\rho c_p)_f c_\mu^{1/4} k_w^{1/2} (\bar{T} - T_w)}{\left(\frac{\sigma_t}{\kappa} \ln(\gamma_w^+) + c_Q(Pr)\right)} \quad (1.53)$$

where $u_\tau = (\tau_w/\rho)^{1/2}$, $\gamma_w^+ = \gamma_w u_\tau/\nu$, $c_Q = 12.5 Pr^{2/3} + 2.12 \ln(Pr) - 5.3$ for $Pr > 0.5$.

In Eq. (1.53), Pr and σ_t are the Prandtl and turbulent Prandtl numbers, respectively, q_w is wall heat flux, u_τ is wall-friction velocity, γ_w is the normal coordinate of the first grid point close to the wall and κ is the von Kármán constant. Further, in Eq. (1.53) E is also a constant, which can accommodate different types of surface. For smooth surfaces, a standard numerical value taken for E is 9.0. The other boundary conditions are the following.

(c) On the symmetry planes:

$$\frac{\partial \bar{u}}{\partial y} = \frac{\partial k}{\partial y} = \frac{\partial \varepsilon}{\partial y} = 0; \quad (1.54)$$

(d) On the periodic boundaries:

$$\bar{u}|_{\text{inlet}} = \bar{u}|_{\text{outlet}}, \quad \bar{v}|_{\text{inlet}} = \bar{v}|_{\text{outlet}}, \quad k|_{\text{inlet}} = k|_{\text{outlet}}, \quad \varepsilon|_{\text{inlet}} = \varepsilon|_{\text{outlet}}, \quad (1.55)$$

$$\theta|_{\text{inlet}} = \theta|_{\text{outlet}} \Leftrightarrow \frac{\bar{T} - \bar{T}_w}{\bar{T}_B(x) - \bar{T}_w} \Big|_{\text{inlet}} = \frac{\bar{T} - \bar{T}_w}{\bar{T}_B(x) - \bar{T}_w} \Big|_{\text{outlet}} \quad (1.56)$$

The bulk mean temperature of the fluid is given by

$$\bar{T}_B(x) = \frac{\int \bar{u} \bar{T} dy}{\int \bar{u} dy} \quad (1.57)$$

Computations are based on the Darcy velocity, the length of structural unit H and the temperature difference $(\bar{T}_B(x) - \bar{T}_w)$ as reference scales.

1.3.2

Periodic Flow

Results for velocity and temperature fields were obtained for different Reynolds numbers. In order to ensure that the flow was hydrodynamically and thermally developed in the periodic cell of Figure 1.1, the governing equations were solved repetitively in the cell, taking the outlet profiles for $\bar{u}$ and θ at the exit and plugging them back at the inlet. In the first run, uniform velocity and temperature profiles were set at the cell entrance for $Pr = 1$ giving $\theta = 1$ at $x/H = 0$. Then, after convergence of the flow and temperature fields, $\bar{u}$ and θ at $x/H = 2$ were used as inlet profiles for a second run, corresponding to solving again the flow for a similar cell beginning in $x/H = 2$. Similarly, a third run was carried out and again outlet results,

this time corresponding to an axial position $x/H = 4$, were recorded. This procedure was repeated several times until $\bar{u}$ and θ did not differ substantially at both inlet and outlet positions, as obtained in Saito and de Lemos (2006) [38].

For the low Re model, the first node adjacent to the wall requires that the nondimensional wall distance be such that $y^+ = u_\tau y \rho / \mu \leq 1$. To accomplish this requirement, the grid needs a great number of points close to the wall leading to computational meshes of large sizes.

1.3.3

Film Coefficient h_i

The determination of h_i is here obtained by calculating, for the unit cell of Figure 1.1, an expression given as

$$h_i = \frac{Q_{\text{total}}}{A_i \Delta T_{\text{ml}}} \quad (1.58)$$

where the overall heat transferred in the cell, Q_{total} , is given by

$$Q_{\text{total}} = A_c \rho \bar{u}_B c_p (\bar{T}_B|_{\text{outlet}} - \bar{T}_B|_{\text{inlet}}) \quad (1.59)$$

and A_i and A_c are presented in Table 1.1. The bulk mean velocity of the fluid is given by

$$\bar{u}_B(x) = \frac{\int \bar{u} dy}{\int dy} \quad (1.60)$$

and the logarithm mean temperature difference, ΔT_{ml} , is defined as

$$\Delta T_{\text{ml}} = \frac{(\bar{T}_w - \bar{T}_B|_{\text{outlet}}) - (\bar{T}_w - \bar{T}_B|_{\text{inlet}})}{\ln[(\bar{T}_w - \bar{T}_B|_{\text{outlet}})(\bar{T}_w - \bar{T}_B|_{\text{inlet}})]} \quad (1.61)$$

Equation (1.59) represents an overall heat balance on the entire cell and Eq. (1.58) associates the heat transferred to the fluid with a suitable temperature difference. As mentioned earlier, Eqs. (1.1) to (1.4) were solved numerically in the unit cell subjected to conditions (1.55) and (1.56). Once fully developed flow and nondimensional temperature fields were achieved, bulk temperatures were calculated according to Eq. (1.57), at both inlet and outlet positions. They were then used to calculate $h_i D / k_f$ using Eqs. (1.58) to (1.61).

Table 1.1 Interface (A_i) and flow (A_c) areas for distinct rod arrangements.

Geometry	A_i	A_c
Square rods – triangular array	$8D$	$H - D$
Elliptic rods – square array	$2\pi\sqrt{0.5(a^2 + b^2)}$	$H - 2b$

1.4

Results and Discussion

1.4.1

Array of Square Rods

Figure 1.3 shows distributed temperature fields for distinct cell porosities. One can see that the lower the porosity (Figure 1.3a), the higher the average fluid temperatures are for the same mass flow through the bed (same Re_D). This is an indication that the transfer of heat from the solid to the fluid phase is enhanced leading to higher value for h_i as ϕ is reduced. Corresponding results for the heat transfer coefficient are plotted in Figure 1.4 for Re_D up to 400. Also plotted in this figure are results computed with Kuwahara *et al.* (2001) [12] correlation, Eq. (1.51), using different porosity values. The figure clearly indicates that both computations show a reasonable agreement. As mentioned, it is also clearly seen from Figure 1.4 that the lower the porosity, the higher the value of the Nusselt number. Increasing of h_i with Re_D is also observed.

Macroscopically developed flow field for $Pr=1$ and $Re_D=10^5$ are presented in Figure 1.5, corresponding to the axial position $x/D=6$ along the longitudinal coordinate (see Figure 1.1). The expression “macroscopically developed” is used herein to account for the fact that periodic flow has been achieved at that axial position. The figure shows the velocity field, streamlines, pressure and turbulent kinetic energy distributions for $\phi=0.65$. The flow impinges on the left face of the obstacles (Figure 1.5a), surrounds the rod faces and forms a weak recirculation bubble past the rod (Figure 1.5b). Pressure increases at the front face of the rod and drastically decreases behind the obstacles, as can be seen from the pressure contours shown in Figure 1.5c. Figure 1.5d illustrates levels of turbulence kinetic energy, which are higher around the rod corners where a strong shear layer is formed. Further downstream of the rods, in the wake region, steep velocity gradients appear due to flow deceleration, increasing there also the local level of turbulence kinetic energy.

Corresponding temperature distribution is shown in Figure 1.6, also for $Re_D=10^5$ and $\phi=0.65$. Colder fluid impinges on the rod left side yielding strong temperature gradients on that face. Downstream of the obstacles, fluid recirculation smoothes temperature gradients and deforms isotherms within the mixing region, which is here more clearly seen with a staggered geometry. When the Reynolds number is sufficiently high, thermal boundary layers cover the rod surfaces indicating that convective heat transfer overwhelms thermal diffusion.

1.4.2

Array of Elliptic Rods

Figure 1.7 presents the temperature fields corresponding to different Re_D and porosities, covering the laminar flow range $100 \leq Re_D \leq 1000$. Inspecting the figure, one can observe that the lower the porosity, the more efficiently heat is added to the fluid. Consequently, values of h_i tend to be higher for lower values of ϕ , in a fashion

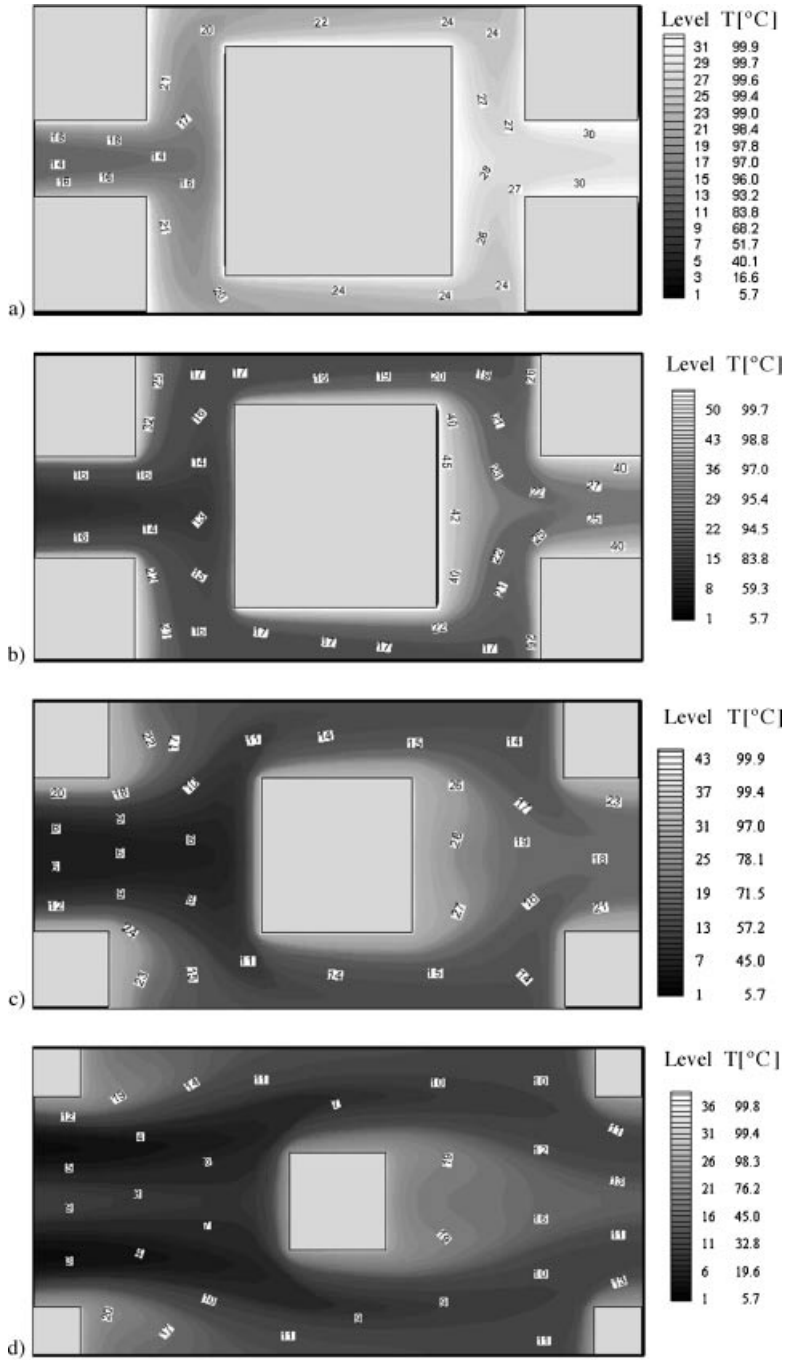


Figure 1.3 Temperature fields in a periodic cell for square rods and $Re_D = 100$; (a) $\phi = 0.44$; (b) $\phi = 0.55$; (c) $\phi = 0.75$; (d) $\phi = 0.90$.

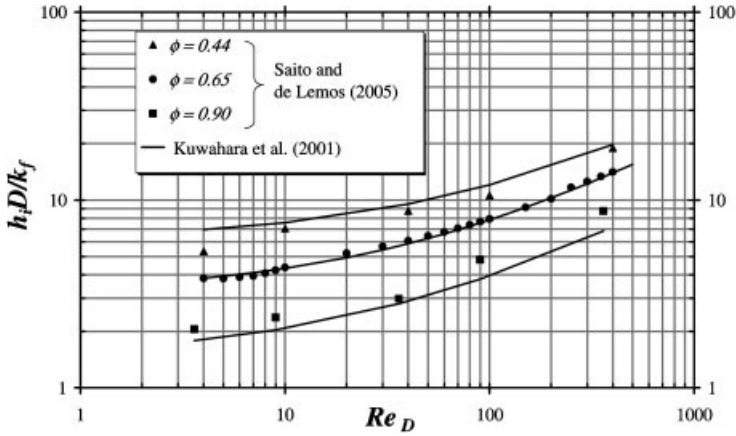


Figure 1.4 Effect of Re_D and ϕ on h_i and comparison with correlation of Kuwahara *et al.* [12] (data from [15]).

similar to what occurred with the square rod case seen above. Also, as Re_D increases, heat is transferred more effectively to the flow, as expected. Figure 1.8 compares integrated h_i values for square and elliptic rods for porosities $\phi = 0.75$ and $\phi = 0.90$. Also shown are results by Kuwahara *et al.* (2001) [12]. It is interesting to note that the more streamlined flow over elliptic rods, which are displaced in an aligned manner, is less effective in promoting heat transfer between phases. Also, the higher the Re_D number, the higher the heat transfer coefficient. Figure 1.9 compiles h_i values as a function of porosity and Re_D up to 1000. As in the case of square obstacles, the lower the porosity the higher the heat transfer rate for the same mass flux across the bed. However, such dependency on ϕ appears to be weaker than in the cases of square rods, if one compares the wider spread of data as porosity varies in Figure 1.4. In addition, as Re_D increases, the effect of ϕ on h_i becomes less pronounced. Also, the figure seems to indicate two distinct regimes, the first one for $Re_D < 100$ and a second for $Re_D > 100$. However, the limited amount of data presented here does not allow more definite conclusions to be drawn.

Results for high Re numbers are considered next. Figure 1.10 shows distributions of pressure, turbulence kinetic energy and temperature fields in the periodic cell of Figure 1.2b, which were obtained at $Re_D = 10^5$ for the cases of $\phi = 0.60$ and $\phi = 0.90$. One can observe that pressure increases at the left face of the rods and decreases behind them, with the surface peak pressure moving towards the stagnation point on the left, along the ellipse horizontal axis, as ϕ increases. The turbulence kinetic energy distribution is presented in Figures 1.10c and d. Levels of k are higher close to the walls and along the converging section of the channel where a strong shear layer prevails. The temperature distribution pattern is presented in Figures 1.10e and f showing that a thermal boundary layer covers most of the surface, possibly indicating that convective heat transfer overwhelms thermal diffusion for the case of high mass flow rates.

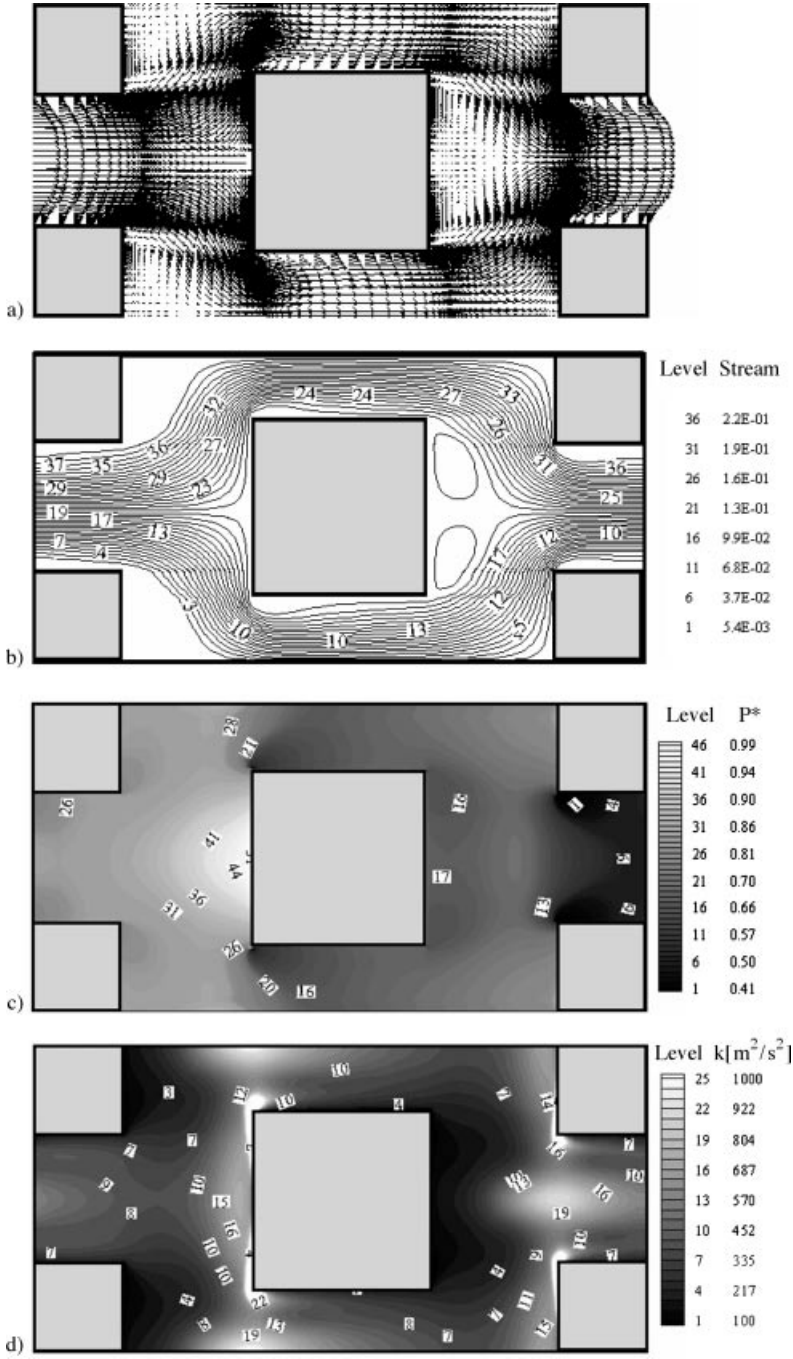


Figure 1.5 Spatially periodic flow and pressure fields, $Re_D = 10^5$ and $\phi = 0.65$;
 (a) vector plot; (b) streamlines; (c) pressure; (d) turbulent kinetic energy.

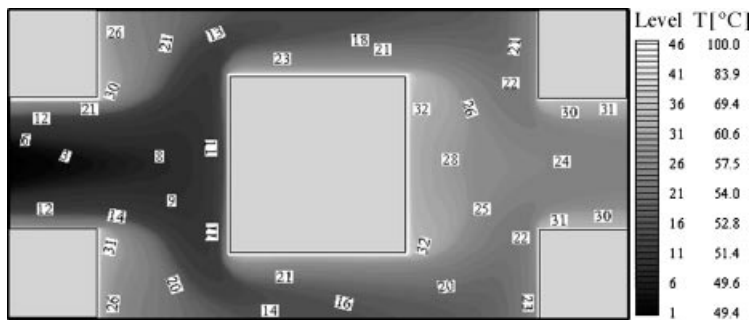


Figure 1.6 Spatially periodic temperature field, $Re_D = 10^5$ and $\phi = 0.65$.

Results for $h_i D/k_f$ are plotted in Figure 1.11 for Re_D up to 10^7 . Also plotted in this figure are results computed with correlation 1.51 by Kuwahara *et al.* (2001) [12] using $\phi = 0.65$. The figure seems to indicate that computations show a reasonable agreement for laminar results. In addition, numerical results for turbulent flow using low and high Re models are also presented in this figure. Differences in the flow pattern between the cases here reported, namely aligned-elliptic rods and staggered-square obstacles, are reflected in the lower heat transfer coefficients for the former case. Sharpe edges of square obstacles, disposed in a triangular arrangement, agitate the fluid in a much stronger fashion than in the case of well-behaved streamlined flow across elliptic tubes.

Figure 1.12 shows numerical results for the interfacial convective heat transfer coefficient for porosities $\phi = 0.65$ and $\phi = 0.90$. Results for $h_i D/k_f$ are plotted for Re_D up to 10^7 comparing the two geometries here analyzed. The figure indicates that the lower the porosity, the higher the ratio $h_i D/k_f$, an effect which is less pronounced when computing the more “unobstructed” flow past the inline-arranged elliptic rods.

1.4.3

Correlations for Laminar and Turbulent Flows

Results for h_i covering both laminar [15] and turbulent flow regimes are plotted in Figure 1.13 along with correlation (1.51) by Kuwahara *et al.* (2001) [12]. Numerical results by Saito and de Lemos (2006) [38] using both low and high Re models are also plotted showing a good overlap of values calculated with both models around $Re_D = 6 \times 10^4$.

Figure 1.14 shows numerical results for the interfacial convective heat transfer coefficient for various porosities and plotted for Re_D up to 10^7 . In order to obtain a correlation for h_i in the turbulent regime, all curves were first collapsed after plotting them in terms of Re_D/ϕ , as shown in Figure 1.15. Next, the least squares technique was applied in order to determine the best correlation, which led to a minimum

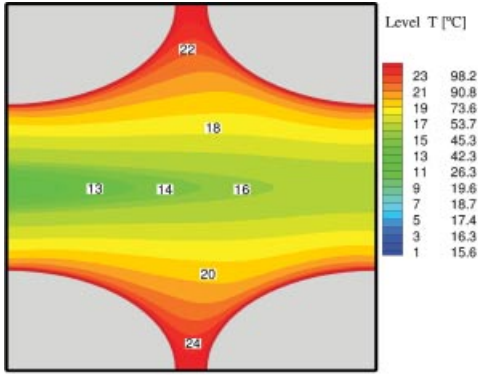
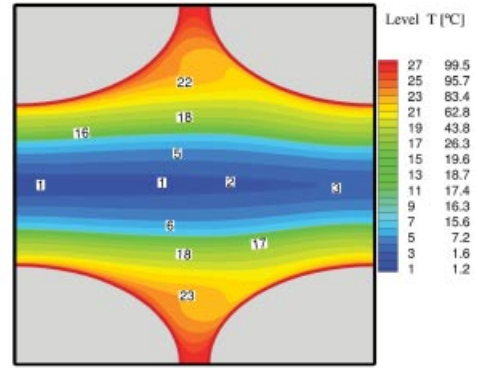
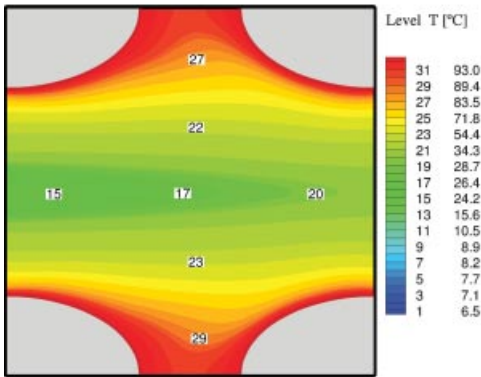
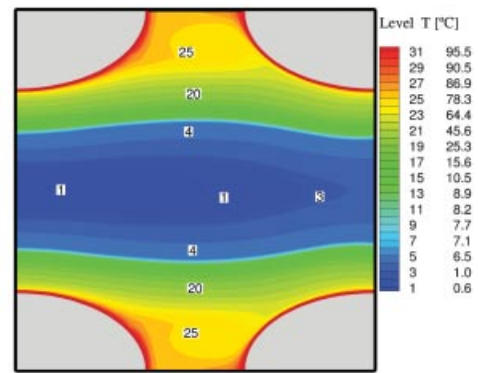
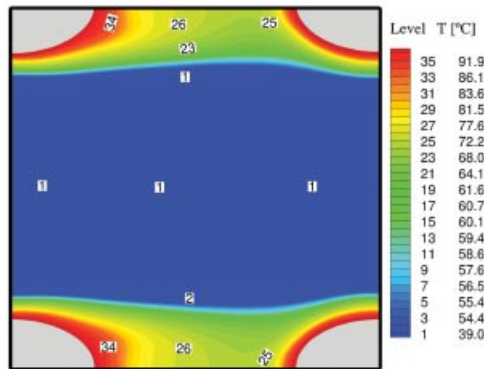
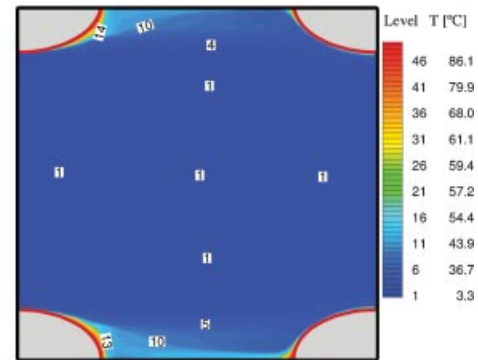
a) $Re_D = 100$ and $\phi = 0.60$ b) $Re_D = 1000$ and $\phi = 0.60$ c) $Re_D = 100$ and $\phi = 0.75$ d) $Re_D = 1000$ and $\phi = 0.75$ e) $Re_D = 100$ and $\phi = 0.90$ f) $Re_D = 1000$ and $\phi = 0.90$

Figure 1.7 Temperature fields in a periodic cell formed by elliptic rods.

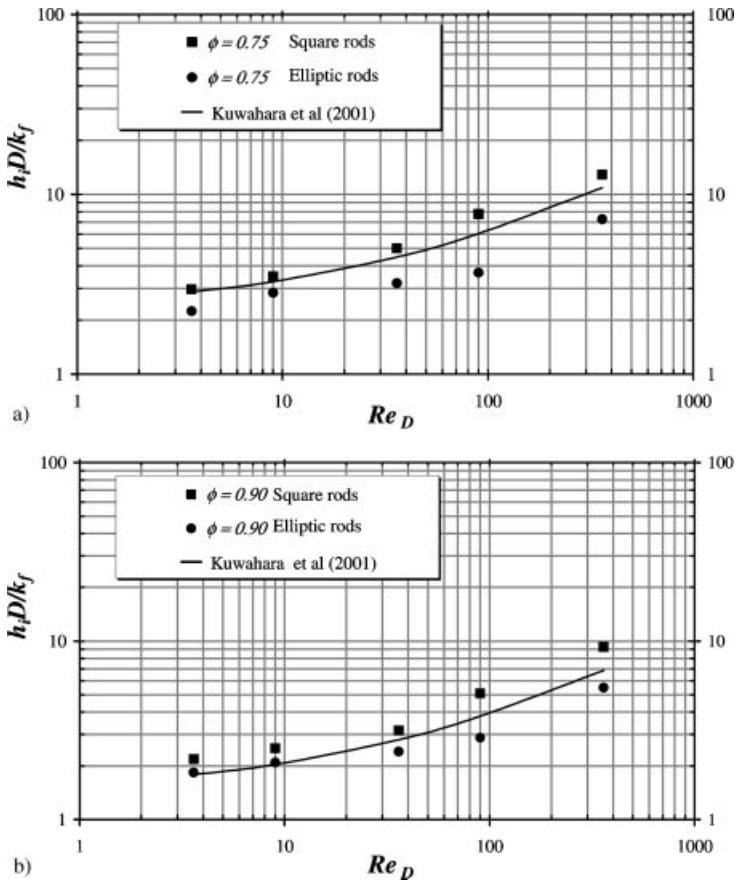


Figure 1.8 Comparison between square rods, elliptic rods and correlation of Kuwahara *et al.* [12] for $\phi = 0.75$ and 0.90 .

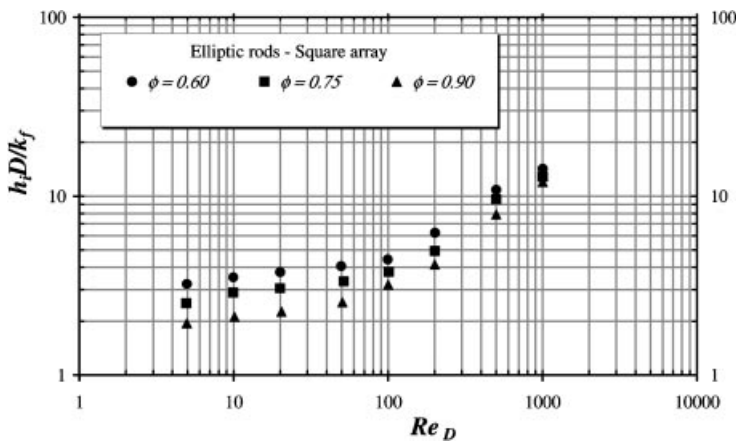


Figure 1.9 Effect of porosity ϕ on h_i for $Pr = 1$ and laminar flow.

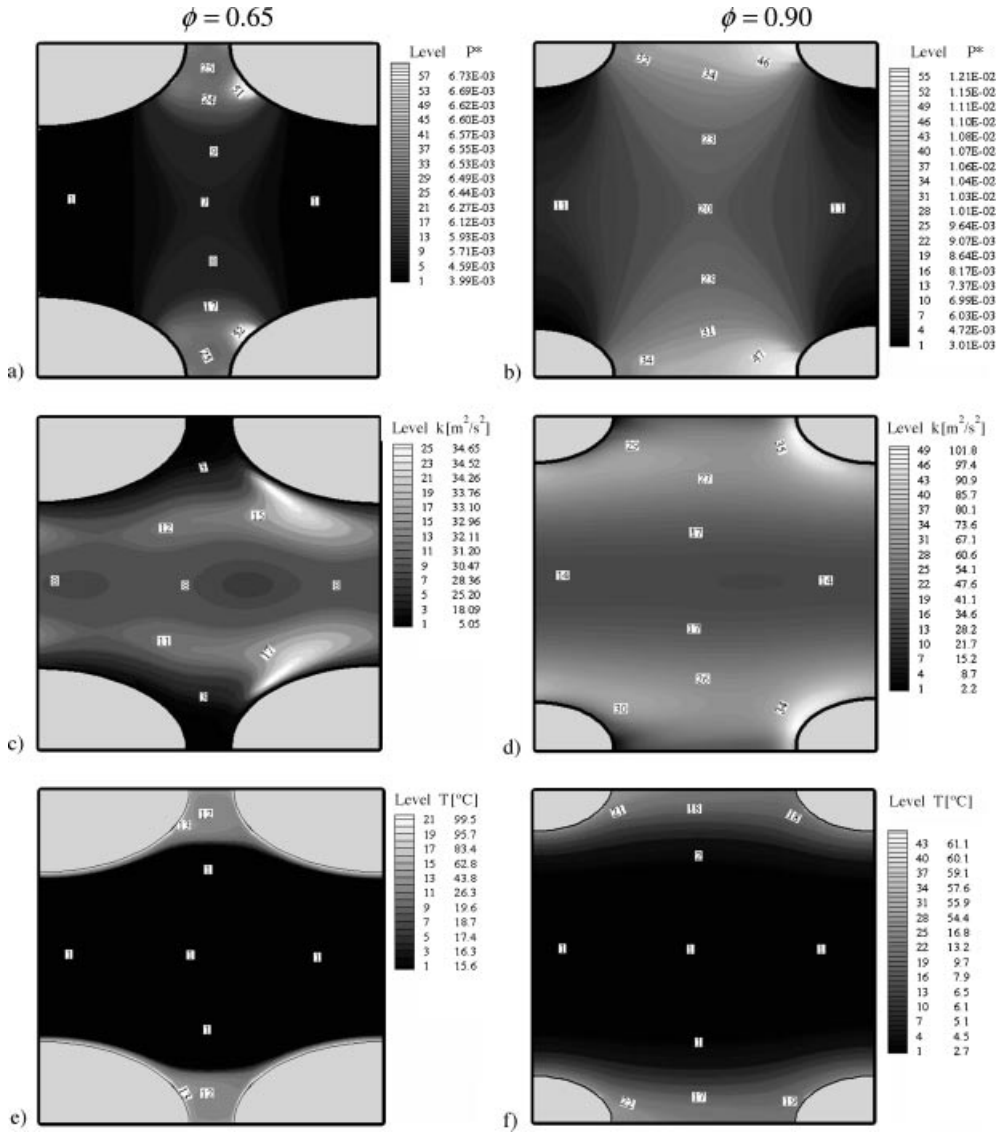


Figure 1.10 Results for elliptic rods, $Re_D = 10^5$:
(a, b) pressure; (c, d) turbulent kinetic energy; (e, f) temperature field.

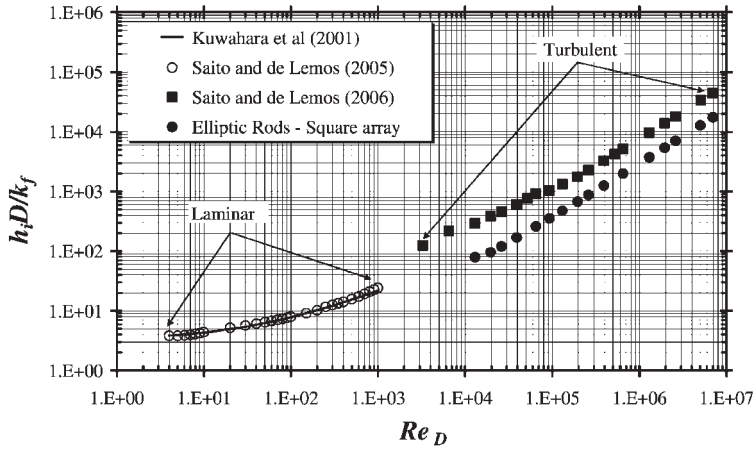


Figure 1.11 Effect of Re_D on h_i for turbulent flow, $Pr = 1$ and $\phi = 0.65$ (data from [12,15,38]).

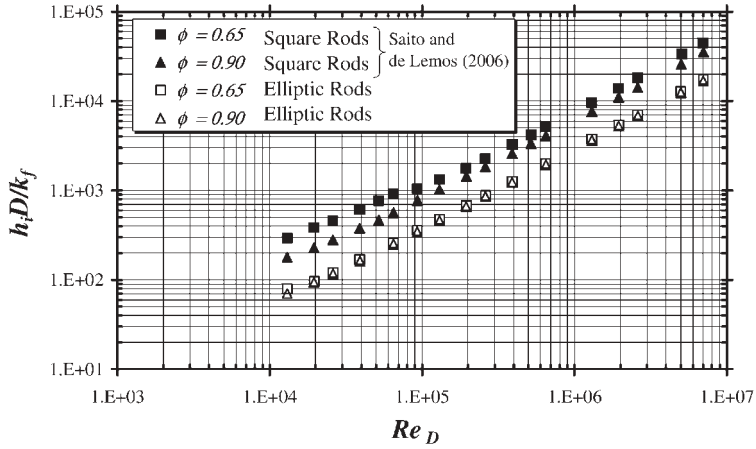


Figure 1.12 Effect of Re_D on h_i for distinct porosities and shapes (data from [38]).

overall error. Thus, the following expression was proposed in Saito and de Lemos (2006) [38]:

$$\frac{h_i D}{k_f} = 0.08 \left(\frac{Re_D}{\phi} \right)^{0.8} Pr^{1/3}; \quad \text{for } 1.0 \times 10^4 < \frac{Re_D}{\phi} < 2.0 \times 10^7, \\ \text{valid for } 0.2 < \phi < 0.9 \quad (1.62)$$

Equation (1.62), which gives the heat transfer coefficient for turbulent flow, is now compared with numerical results obtained with low and high Re models. Such a

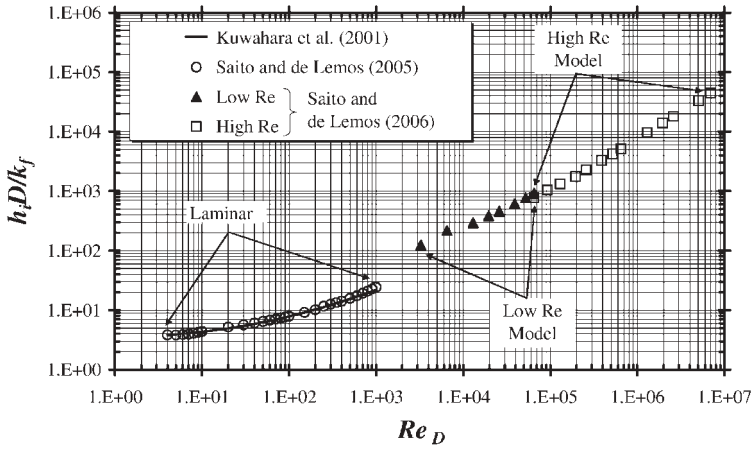


Figure 1.13 Effect of Re_D on h_i for turbulent flow, $Pr = 1$ and $\phi = 0.65$ (data from [12,15,38]).

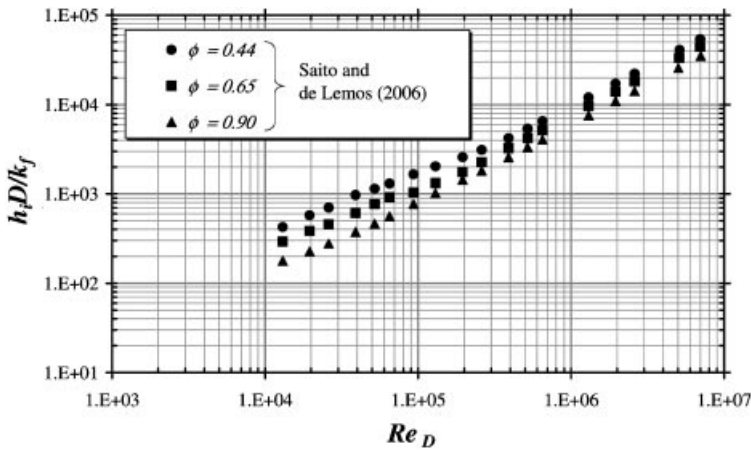


Figure 1.14 Effect of porosity on h_i for $Pr = 1$, square rods (data from [38]).

comparison is presented in Figure 1.16, which also shows computations using correlations given by Zhukauskas (1972) [57] and Wakao *et al.* (1979) [56], Eqs. (1.49) and (1.50), respectively. Table 1.2 summarizes correlations referred to in this chapter, through which the heat transfer coefficient h_i in porous media can be determined.

Finally, one can say that the agreement between the correlations in the literature and the numerical simulations here reported stimulates further investigation on this subject, contributing towards the building of a more general expression for the interfacial heat transfer coefficient for porous media.

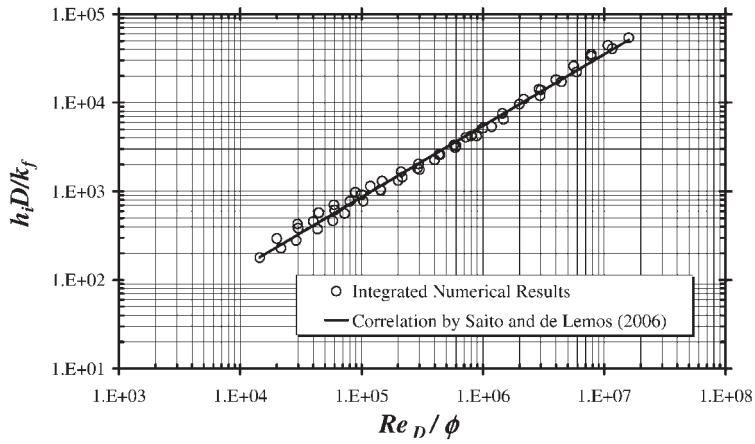


Figure 1.15 Scaled numerical results and comparison with correlation (1.62) by Saito and de Lemos [38].

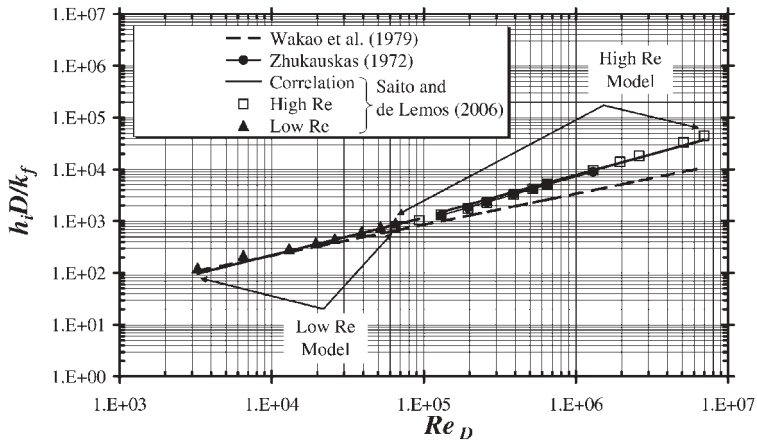


Figure 1.16 Comparison of integrated numerical results for $\phi = 0.65$ and correlations from [38,56,57].

Table 1.2 Correlations for interfacial heat transfer coefficient.

Correlation	Validity	Eq.	Ref.
$\frac{h_i D}{k_f} = 0.022 Re_D^{0.84} Pr^{0.36}$	$2 \times 10^5 < Re_D < 2 \times 10^6$	(1.49)	[56]
$\frac{h_i D}{k_f} = 2 + 1.1 Re_D^{0.6} Pr^{1/3}$	—	(1.50)	[56]
$\frac{h_i D}{k_f} = \left(1 + \frac{4(1-\phi)}{\phi}\right) + \frac{1}{2}(1-\phi)^{1/2} Re_D Pr^{1/3}$	Laminar flow, $0.2 < \phi < 0.9$	(1.51)	[12]
$\frac{h_i D}{k_f} = 0.08 \left(\frac{Re_D}{\phi}\right)^{0.8} Pr^{1/3}$	$1.0 \times 10^4 < Re_D / \phi < 2.0 \times 10^7$ $0.2 < \phi < 0.9$	(1.62)	[38]

1.5

Conclusions

A computational procedure for determining the convective coefficient of heat exchange between the porous substrate and the working fluid for a porous medium was detailed. As a result, macroscopically uniform laminar and turbulent flows through a periodic cell formed by square and elliptic rods were computed. Quantitative agreement was obtained when comparing laminar results herein with simulations by Kuwahara *et al.* (2001) [12]. For turbulent flows, low and high Reynolds turbulence models were employed in order to obtain the interfacial heat transfer coefficient. Correlations for determining the heat transfer coefficient were compared. Ultimately, it is expected that a more general correlation for h_i be obtained to be used in conjunction with more realistic two-energy equation models.

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2

Effective Thermal Properties of Hollow-Sphere Structures: A Finite Element Approach

Andreas Öchsner and Thomas Fiedler

2.1

Introduction

2.1.1

Finite Element Method and Heat Transfer Problems

Scientists and engineers in academia and industry have in recent years become very conversant with numerical techniques of analysis. These techniques are based on the approximate solution of an equation or a set of equations describing a physical problem. From a mathematical point of view, physical problems are described by differential equations or by integral expressions. Thus, the numerical approach seeks to determine the spatial distribution of one or more dependent variables such as temperature, concentration or displacement in a given domain. The first widely known approximation approach was the finite difference method [1,2] which approximates the governing equations of a field problem using local expansions for the variables, generally truncated Taylor series. This technique can be interpreted as a special case of the more general weighted residual method which is applied in Section 2.2.2 to derive the principal finite element equation.

The finite element method (FEM) has attracted the attention of analysts largely due to its property of discretizing a continuous system into a series of *finite elements*, which can be associated with physical parts. The single elements 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.

The pioneering works on finite element methods started in the early 1950s in the aerospace industry (Boeing) where M.J. (Jon) Turner “created” the FEM in everyday use. During this time, only large industrial companies such as in the aerospace industry were able to afford mainframe computers. Four academicians, i.e. J.H. Argyris, R.W. Clough, H.C. Martin and O.C. Zienkiewicz, were largely responsible for the “technology transfer” from the aerospace industry to a wider range of

engineering applications during the 1950s and 1960s. The first three learned the method from Turner directly or indirectly. As a consultant to Boeing in the early 1950s, Argyris at Imperial College, received reports from Turner's group. Clough and Martin, junior professors at the University of California, Berkeley, and the University of Washington, respectively, spent "faculty internship" summers at Turner's group during 1952 and 1953. The result of this seminal collaboration was a celebrated paper [3], widely considered the start of the present FEM. Clough baptised the method in 1960 [4] and went on to form at Berkeley the first research group to propel the idea into civil engineering applications. Olek C. Zienkiewicz, originally an expert on finite difference methods, was convinced in 1964 by Clough to try FEM. He went on to write the first textbook on the subject in 1967 [5] and to organize another important civil engineering research group in the University of Wales at Swansea. Other important works were carried out at MIT in Cambridge, MA and the University of Stuttgart in Germany.

The existing literature on finite elements is by now very extensive and encompasses all types of common field problems such as structural mechanics, heat transfer, fluid flow and acoustics. Mackerle estimated in 1995 [6] that approximately 380 books, 400 conference proceedings and 56 000 papers (excluding papers on fluid mechanics) were published. Furthermore, he noted that at present about 3800 papers are published annually. As standard reference books on finite elements, one may cite, among others, the three-volume textbook by Zienkiewicz and Taylor [7], the textbooks by Bathe [8], by Hughes [9] and by Cook et al. [10]. Several specialized books are devoted to the topic of finite elements and heat transfer [11–15] and the bibliography article by Mackerle [16] cites 210 publications related to finite elements and heat transfer analyses.

As in the case of existing literature, there is a huge number of finite element codes ranging from simple academic programs to commercially available general purpose programs. Some of the common commercial codes used in industry as well as in academia are NASTRAN (Richard H. MacNeal, Robert Schwendler), ANSYS (John Swanson), MARC (Pedro Marcal), ABAQUS (David Hibbitt) and ADINA (Klaus-Jürgen Bathe).

Nowadays, commercial finite element programs are quite powerful and user friendly codes are available for all platforms of operating systems. However, reliable results can only be obtained when the user of such codes understands the problem, how to model it, the behavior of finite elements, the assumptions and limitations of the code, and when the analyst is able to check for errors at all stages. It is not necessary that the end-user understands in detail all procedures and routines, but incorrect results, which may cause serious damage such as production delay, redesign or even collapse, can be avoided only by those who understand the basic ideas and single steps of the FEM.

This chapter aims to give a fundamental introduction into the finite element method for heat *conduction* problems, i.e. how the method is derived, how elements are formulated and how they work. Other mechanisms of heat transfer, i.e. thermal radiation and thermal convection, are covered in other chapters of this book. This theoretical part should impart the basic knowledge on the method which is required

for a sensible application of numerical codes. For simplicity of notation, the method is derived for plane two-dimensional geometries. In contrast to simple one-dimensional examples, the plane approach comprises many particularities which can be easily transferred to the general three-dimensional case. In the second part of the chapter, the finite element method will be applied to determine the effective thermal conductivity of hollow-sphere structures (HSS). This special class of cellular metals will be generally introduced in the next section.

2.1.2

Hollow-Sphere Structures in the Context of Cellular Metals

The concept of porous and cellular metals first emerged in the beginning of the 1970s [17–19]. The basic idea seeks to imitate the cellular structure of high-performance lightweight structures in nature such as the human osseous structure and can therefore be related to the field of bio-inspired research. A closely related approach has already been successfully brought into application in both the aviation industry [20,21] and the space industry [22,23] through the use of hexagonal honeycomb structures in sandwich cores.

Nowadays, foams made of polymeric materials are widely used in all fields of technology. For example, Styrofoam[®] and hard polyurethane foams are widely used as packaging materials. Other typical application areas of polymeric foams are the field of heat and sound absorption. During the last few years, techniques for the manufacturing of novel cellular and porous metals have been developed [24,25]. These materials exhibit a high potential for future oriented applications due to their specific properties.

By definition, cellular metals are materials with high porosity which are divided into distinct cells. The boundaries of these cells are made of solid metal, while the internal regions are air cavities. Cellular metals therefore exhibit densities which are typically below 10% of their corresponding base metal. This porosity can be quantified by the relative volume V_{rel} which is the volume occupied by the base material divided by the total volume of the structure. Two special cases of cellular metals are metallic foams and sponges. Metallic foams like Alporas[®] (Figure 2.1a) originate from a liquid and are characterized by closed cells. Metallic sponges such as M-Pore[®] (Figure 2.1b) are characterized by an interconnected porosity of open cells. In contrast to *cellular* metals, *porous* metals contain a multitude of microscopic pores and the densities of these materials are in the range of their base material(s). It should be mentioned here that the definitions of metallic foam, sponge and porous metals are not mutually exclusive.

Well-known advantages of cellular metals are their high ability for energy adsorption [26–28], good damping behavior [29–31], sound absorption [32], excellent heat insulation [33–35] and a high specific stiffness [36–38]. The combination of these properties opens a wide field of potential applications, e.g. in automotive, aviation or the space industry [39–41]. However, despite more than 30 years of intensive scientific research, few industrial applications of these technologies can be found. Essential limiting factors for their utilization are unevenly distributed material

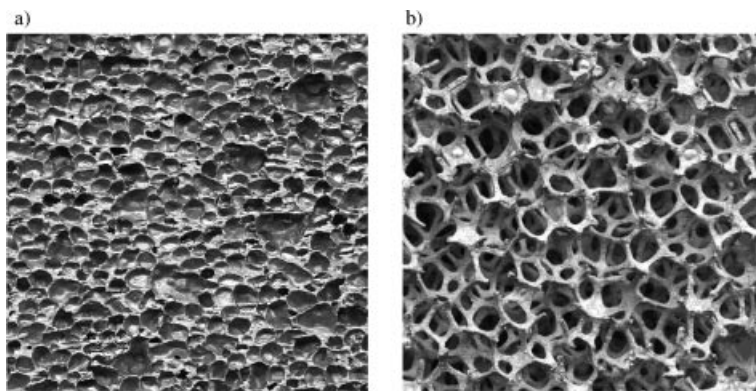


Figure 2.1 Cellular metals: (a) Alporas[®] aluminum foam; (b) M-Pore[®] aluminum sponge.

parameters [27,28] and relatively high production costs. Less variation in the physical properties can be achieved with lattice block materials [44,45]. These structures are manufactured by investment casting and therefore exhibit a well-defined, reproducible geometry (periodic 3D truss structure). However, this manufacturing technology is only able to produce open-celled structures. Further limitations are high costs and anisotropic properties caused by the microstructure orientation.

Metallic hollow-sphere structures (MHSS) are a new group of cellular metals characterized by easily reproducible geometry and therefore consistent mechanical and physical properties. A new powder metallurgy-based manufacturing process enables the production of metallic hollow spheres of defined geometry [46]. This technology brings a significant reduction in costs in comparison to earlier applied galvanic methods and all materials suitable for sintering can be applied. EPS (expanded polystyrol) spheres are coated with a metal powder–binder suspension by turbulence coating. The green spheres produced can either be sintered separately to manufacture single hollow spheres or be pre-compacted and sintered in bulk (Figure 2.2) thus creating sintering necks between adjacent spheres [47]. Depending on the parameters of the sintering process the microporosity of the sintered cell wall can be adjusted. In a subsequent debinding process, the EPS spheres are pyrolyzed. The increase of the carbon content of the sintered metal by the diffusion of the incinerated binder and polymer causes degradation of mechanical properties and corrosion resistance. Special reducing processes are required to reduce this effect [48].

Various joining technologies such as sintering, soldering and adhering can be used to assemble the single hollow spheres to interdependent structures [49,50]. Adhering is the most economic way of joining and therefore is attractive for a wide range of potential applications. Another important advantage is the possible utilization of the mechanical behavior and morphology of the adhesive layer as a further design parameter for the optimization of the structure's mechanical properties for specific applications. Figure 2.3 shows two different types of adhesively bonded MHSS.

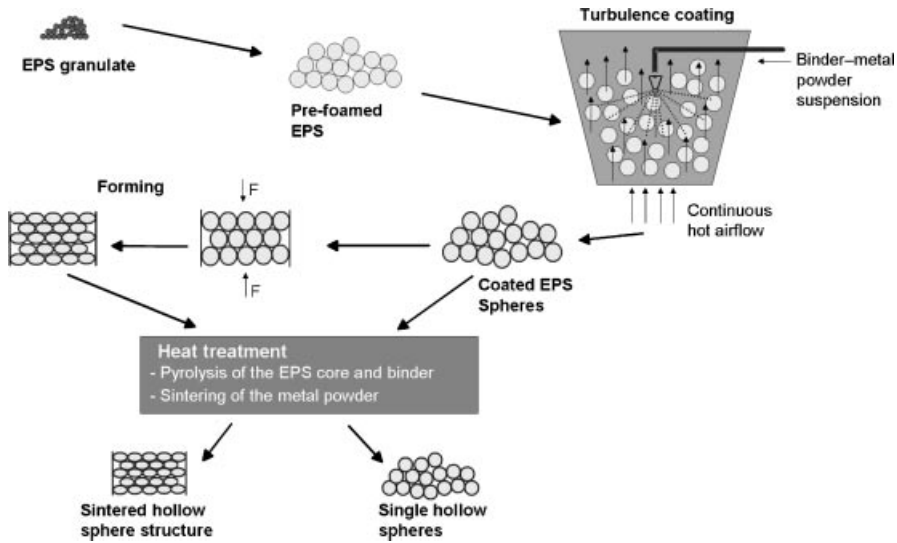


Figure 2.2 Manufacturing process of metallic hollow-sphere structures.

In the case of syntactic morphology, the hollow spheres are completely embedded within the adhesive matrix as in the case of classical fiber-reinforced plastics. In contrast, the adhesive is concentrated at the contact points of neighboring spheres for partial MHSS. Consequently, partial MHSS also exhibit interconnected porosity.

Cellular metals exhibit a multitude of interesting properties. Based on these characteristics, highly integrated applications can be created. First, due to the high porosity of MHSS, the material is able to compress at high strains. The typical stress-strain diagram of a MHSS reveals a stress plateau which characterizes the ability of the structure to absorb energy at a low stress level and high strains. This

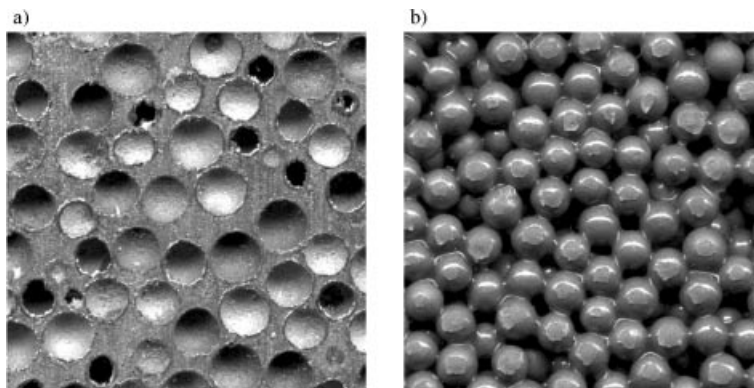


Figure 2.3 Adhesively bonded metallic MHSS:
(a) Cross-section of a syntactic MHSS; (b) partial morphology.

property enables the application of MHSS in energy-absorbing structures, e.g. crash elements in the automotive industry [40]. Another clear attribute of cellular structures is the damping of mechanic and acoustic oscillations. In conjunction with low density, this property suggests the utilization in parts where high accelerations occur. Oscillations can be damped and energy consumption can be reduced due to the small amount of accelerated mass. The significant potential of hollow sphere composite structures in machine tools has already been demonstrated [51]. Furthermore, cellular metals can act as sound suppressors and acoustic insulators. Cellular metals also exhibit a low thermal conductivity in comparison to their metallic base materials. In particular, adhesively bonded MHSS show very low thermal conductivities, due to the insulating effect of the adhesive matrix between the metallic shells of the spheres. Consequently, MHSS can be applied as thermal insulators [52,53]. Other approaches aim for the utilization of metallic sponges inside heat exchangers [54,55]. However, since MHSS exhibit only low (partial morphology) or no (syntactic morphology) interconnected porosity, they possess a high flow resistance and are not suitable for such applications.

Sandwich structures are essential machine elements in lightweight construction and a typical field of (possible) industrial application of cellular metals. In particular, aluminum sandwich constructions have been recognized as a promising concept for structural design of lightweight transportation systems such as aircraft [56,57], high-speed trains [58,59] and fast ships [60,61]. The classic definition of a sandwich structure in lightweight applications is a composite where a light core material is enclosed by two or more layers of a fully dense material. The basic principle of sandwich structures is for two strong face sheets to bear the applied loads while the core acts as a spacer which retains the face sheets in position by carrying shear stresses. Therefore, the core must be stiff enough in the direction perpendicular to the faces to ensure that they remain the correct distance apart and exhibit sufficient shear stiffness to ensure that when the panel is bent the faces do not slide over each other. The core material does not need to reach the mechanical performance of the face sheets and typically low-density materials are applied [62]. Nowadays, the industrial standards for sandwich cores are honeycomb structures which exhibit excellent stiffness at very low densities. However, the processing of honeycomb structures, especially as a core between curved face sheets, is complex and therefore increases the manufacturing costs. Furthermore, honeycomb structures possess poor resistance to contact and impact loads [63–65] and exhibit anisotropic properties. This shows that there is a necessity for new innovative core materials.

In Figure 2.4a an M-Pore[®] aluminum sponge is applied as core material. This commercially available material is characterized by very high porosity and therefore low density. Figure 2.4b shows the Alporas[®] aluminum foam with closed cells and a slightly higher densities but also improved mechanical properties. In Figures 2.4c and d partial and syntactic MHSS cores are shown. For industrial applications these core materials have to be able to compete with classic honeycomb structures (Figure 2.4e). The benefits of cellular metal as sandwich cores, relative to competing concepts, arise primarily in curved configurations where the isotropy of the material is advantageous [26,36,66]. Due to the multifunctional properties of

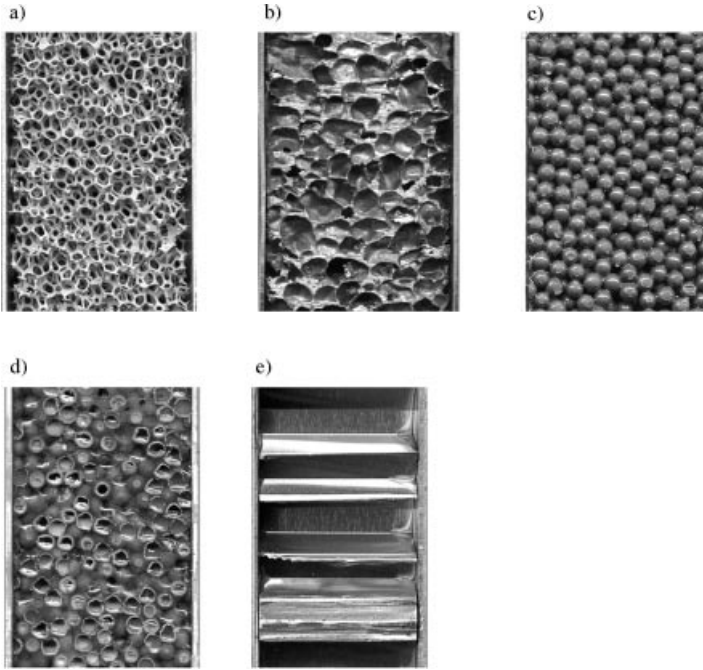


Figure 2.4 Sandwich structures containing different core materials: (a) M-Pore[®], (b) Alporas[®], (c) partially adhesively bonded MHSS, (d) syntactic adhesively bonded MHSS, (e) honeycomb structure.

cellular metals the selection of the optimum core material requires the consideration of all characteristics with relevance to the intended application. Furthermore, the potential utilization in safety-relevant fields puts high demands on the predictability and stability of their properties. In the scope of this work, MHSS are numerically analyzed from the viewpoint of their application as thermal insulators in sandwich panels. Special focus is given to adhesively bonded MHSS. This joining technology allows flexible processing and the adjustment of the properties of the composite by the selection of different adhesives.

2.2

Finite Element Method

2.2.1

Basics of Heat Transfer

Heat conduction analysis is based on Fourier's law (conduction rate equation)

$$\mathbf{q} = -k \nabla T \quad (2.1)$$

where $\mathbf{q} = \{q_x, q_y\}^T$ is the heat flux vector and $\nabla T = \left\{ \frac{\partial T}{\partial x}, \frac{\partial T}{\partial y} \right\}^T$ is the temperature gradient vector which is generated by the Nabla operator $\nabla = \left\{ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right\}^T$. The continuum conductivity matrix $\mathbf{k}$ is given for an anisotropic material as

$$\mathbf{k} = \begin{bmatrix} k_x & k_{xy} \\ k_{yx} & k_y \end{bmatrix} \quad (2.2)$$

which reduces for isotropic materials to

$$\mathbf{k} = k \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (2.3)$$

Fourier's law is not an expression which can be derived from first principles (conservation of energy). It is instead a generalization based on experimental evidence and defines an important material property, the thermal conductivity. In addition, it is a vector expression stating that the heat flux is normal to an isotherm and in the direction of decreasing temperature.

To solve a heat conduction problem means to determine the temperature field $T = T(x, y, t)$ in its spatial and temporal dependency. Then the heat flux field can be determined according to Fourier's law (2.1). The unknown temperature field is obtained by solving a partial differential equation (PDE), the so-called heat diffusion equation (HDE). This PDE can be obtained by applying the first law of thermodynamics to a differential control volume which gives after some transformations the continuity equation of thermodynamics. Combining the continuity equation with Fourier's law and introducing a third law describing the relationship between temperature and energy gives the heat diffusion or heat conduction equation in its general form as [67,68]

$$\rho c_p \frac{\partial T}{\partial t} = \nabla^T (\mathbf{k} \nabla T) + \dot{q} \quad (2.4)$$

where ρ is the mass density, c_p the specific heat at constant pressure, t the time and $\dot{q}$ the energy rate per unit volume, i.e. a heat source or sink.

2.2.2

Weighted Residual Method

Let us consider in the following the special case of the steady-state HDE ($\partial T / \partial t = 0$) where no sources or sinks are present ($\dot{q} = 0$):

$$\nabla^T (\mathbf{k} \nabla T_0) = 0 \quad (2.5)$$

The basic idea of the weighted residual method [69] consists of multiplying the partial differential equation (2.5) with a weighting function w and to demand that the entire integral vanishes over the whole domain. For the true solution T_0 , this expression is independent of the weighting function and always fulfilled. Substituting

the exact solution T_0 by an approximate solution¹⁾ T produces a “residual” or “error” function R such that

$$R = \nabla^T(\mathbf{k}\nabla T) \neq 0 \quad (2.6)$$

This error will be distributed according to the scalar weighting function $w = w(x, y)$ and the integral over the entire two-dimensional domain $\Omega = (x, y)$ will be forced to be zero in a certain average sense:

$$\int_{\Omega} w(\nabla^T(\mathbf{k}\nabla T)) d\Omega = \int_{\Omega} w R d\Omega = 0. \quad (2.7)$$

Equation (2.7) is known as the so-called inner product while the original statement, i.e. Eq. (2.5), is referred to as the strong formulation or classical form. The so-called weak formulation, i.e. where the order of the differential operator is the same for w and T , can be derived by application of the Green–Gauss theorem [70]:

$$\int_{\Omega} w \nabla^T(\mathbf{k}\nabla T) d\Omega = \int_{\Gamma} w(\mathbf{k}\nabla T)^T \mathbf{n} d\Gamma - \int_{\Omega} (\nabla^T w)(\mathbf{k}\nabla T) d\Omega = 0 \quad (2.8)$$

$$\int_{\Omega} (\nabla^T w)(\mathbf{k}\nabla T) d\Omega = \int_{\Gamma} w(\mathbf{k}\nabla T)^T \mathbf{n} d\Gamma \quad (2.9)$$

The weak formulation (2.9) forms the basis for the derivation of the principal finite element equation. Other numerical methods, e.g. the boundary element method, require further integration of the weak formulation which results in the so-called inverse formulation where the differential operator is completely shifted to the weighting function. All classic approximation methods can be derived based on the weighted residual method. The degree of integration and the choice of the weighting function w defines finally which method is obtained [69].

2.2.3

Discretization and Principal Finite Element Equation

The basic idea of the finite element method is to approximate the unknown temperature T not in the entire domain Ω as given in Eq. (2.9) but in a subdomain Ω_e , i.e. a so-called finite element, by an expansion

$$T_e = \mathbf{N}_e^T \mathbf{T}_{e,n} = \{N_1 \quad N_2 \quad \dots \quad N_n\} \begin{Bmatrix} T_{e,1} \\ T_{e,2} \\ \vdots \\ T_{e,n} \end{Bmatrix} \quad (2.10)$$

¹⁾ For simplicity, the variable T will be used in the following for the approximate solution. This

variable should not be confused with the real continuum temperature T of Section 2.2.1.

where N_n are the shape functions prescribed in terms of independent variables (such as the spatial coordinates) and all or most of the nodal temperatures $T_{e,n}$ are unknown. Index n denotes the number of nodes. To derive the FEM, the weighting function w is approximated within an element in a similar manner as the temperature (this approach is also known as the Galerkin method):

$$w = \delta T_{e,n}^T \mathbf{N}_e = \begin{Bmatrix} \delta T_{e,1} & \delta T_{e,2} & \dots & \delta T_{e,n} \end{Bmatrix} \begin{Bmatrix} N_1 \\ N_2 \\ \vdots \\ N_n \end{Bmatrix} \quad (2.11)$$

where $\delta T_{e,n}$ are arbitrary temperatures and n is the number of unknowns entering the system. Using these two field approximations, the left-hand side (LHS) of Eq. (2.9) can be written as

$$\int_{\Omega_e} (\nabla^T (\delta T_{e,n}^T \mathbf{N}_e)) (k \nabla (\mathbf{N}_e^T T_{e,n})) d\Omega_e \quad (2.12)$$

where the vectors $\delta T_{e,n}$ and $T_{e,n}$ are not a function of the spatial coordinates and thus can be considered as constants with respect to the Nabla operator ∇ . Consequently, these temperature vectors can be taken out of the brackets to give

$$\delta T_{e,n}^T \int_{\Omega_e} (\nabla^T \mathbf{N}_e) (k \nabla \mathbf{N}_e^T) d\Omega_e T_{e,n} = \delta T_{e,n}^T \mathbf{K}_e T_{e,n} \quad (2.13)$$

The matrix $\mathbf{K}_e$ is the thermal conductivity matrix and is of dimension $[n \times n]$. Application of the Nabla operator to the vector of shape functions gives the following statement

$$\mathbf{K}_e = \int_{\Omega} \left\{ \frac{\partial \mathbf{N}_e}{\partial x} \frac{\partial \mathbf{N}_e}{\partial y} \right\} k \left\{ \frac{\partial \mathbf{N}_e^T}{\partial x} \frac{\partial \mathbf{N}_e^T}{\partial y} \right\} d\Omega_e \quad (2.14)$$

or with the single shape functions in more detail as

$$\mathbf{K}_e = \int_{\Omega_e} \left\{ \begin{Bmatrix} \frac{\partial N_1}{\partial x} \\ \frac{\partial N_2}{\partial x} \\ \vdots \\ \frac{\partial N_n}{\partial x} \end{Bmatrix} \begin{Bmatrix} \frac{\partial N_1}{\partial y} \\ \frac{\partial N_2}{\partial y} \\ \vdots \\ \frac{\partial N_n}{\partial y} \end{Bmatrix} \right\} k \left\{ \begin{Bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \dots & \frac{\partial N_n}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \dots & \frac{\partial N_n}{\partial y} \end{Bmatrix} \right\} d\Omega_e \quad (2.15)$$

The integration over the subdomain Ω_e is approximated by numerical integration (see next section). To this end, the coordinates (x, y) are transformed to the unit space (ξ, η) where each coordinate ranges from -1 to 1 . In the scope of this coordinate transformation, attention must be paid to the derivatives. For example, the derivative of the shape functions with respect to the x -coordinate is transformed in the following way:

$$\frac{\partial N_i}{\partial x} \rightarrow \frac{\partial N_i}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_i}{\partial \eta} \frac{\partial \eta}{\partial x}, \quad i = 1, \dots, n \quad (2.16)$$

Introducing these new derivatives gives the element conductivity matrix

$$K_e = \int_{\Omega'_e} \left\{ \frac{\partial N_e}{\partial \xi} \quad \frac{\partial N_e}{\partial \eta} \right\} \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} \mathbf{k} \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\ \frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} \end{bmatrix} \begin{Bmatrix} \frac{\partial N_e^T}{\partial \xi} \\ \frac{\partial N_e^T}{\partial \eta} \end{Bmatrix} d\Omega'_e \quad (2.17)$$

where $d\Omega'_e = J d\xi d\eta$. The last equation can be written in the following compact form:

$$K_e = \int_{\Omega'_e} \mathbf{B} \mathbf{k} \mathbf{B}^T d\Omega'_e \quad (2.18)$$

where $\mathbf{B} = \left\{ \frac{\partial N_e}{\partial \xi} \quad \frac{\partial N_e}{\partial \eta} \right\} \mathbf{J} = \nabla' N_e^T \mathbf{J}$ is the temperature gradient matrix. Multiplying the gradient vector of the shape functions, $\nabla' N_e^T$, with the matrix of geometrical derivatives, $\mathbf{J}$, gives a row vector of dimension $[1 \times 2]$. However, each of the elements of this vector is again a column vector with n elements and the product can finally be regarded as a matrix of dimension $[n \times 2]$:

$$\mathbf{B} = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_1}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_1}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_1}{\partial \eta} \frac{\partial \eta}{\partial y} \\ \frac{\partial N_2}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_2}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_2}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_2}{\partial \eta} \frac{\partial \eta}{\partial y} \\ \vdots & \vdots \\ \frac{\partial N_n}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_n}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_n}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_n}{\partial \eta} \frac{\partial \eta}{\partial y} \end{bmatrix} \quad (2.19)$$

Multiplying $\mathbf{B}$ with $\mathbf{B}^T$ or $\mathbf{k} \mathbf{B}^T$ gives finally the element conductivity matrix which is of dimension $[n \times n]$. Summarizing, we can conclude that the evaluation of the element conductivity matrix K_e comprises the following steps:

- determination of the temperature gradient matrix $\mathbf{B}$,
- triple matrix product $\mathbf{B} \mathbf{k} \mathbf{B}^T$,
- numerical integration.

To evaluate the right-hand side (RHS) of the weak statement according to Eq. (2.9), we introduce the field approximation of the weighting function according to $w = \delta T_{e,n}^T \mathbf{N}_e$:

$$\int_{\Gamma_e} (\delta T_{e,n}^T \mathbf{N}_e) (\mathbf{k} \nabla T)^T \mathbf{n} d\Gamma_e \quad (2.20)$$

Since $\delta T_{e,n}^T$ can be cancelled with the LHS of Eq. (2.13), we get

$$\mathbf{F}_e = \int_{\Gamma_e} \mathbf{N}_e (\mathbf{k} \nabla T)^T \mathbf{n} d\Gamma_e \quad (2.21)$$

which needs to be evaluated for each node along the element boundary Γ_e . The vector $\mathbf{F}_e$ is the element vector of externally applied equivalent nodal loads. Equations (2.18) and (2.21) can be combined on the elemental level to the so-called principal finite element equation:

$$\mathbf{K}_e T_{e,n} = \mathbf{F}_e \quad (2.22)$$

2.2.4

Four-Node Planar Bilinear Quadrilateral (Quad4)

As a typical simple element representative, a four-node, isoparametric, arbitrary quadrilateral (Quad4) is discussed in the following. This element can be used for planar (as well as 3D) heat transfer applications. As this element uses bilinear shape functions, the thermal gradients tend to be constant throughout the element. The node numbering must follow the right-hand convention (Figure 2.5).

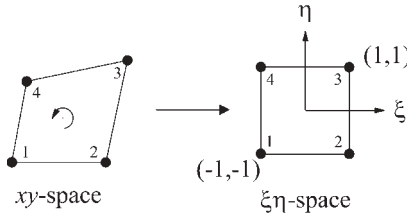


Figure 2.5 Heat transfer quadrilateral element in Cartesian and unit space.

In this 2D case, the temperature gradient matrix is given by

$$\mathbf{B} = \left\{ \frac{\partial \mathbf{N}_e}{\partial \xi} \frac{\partial \mathbf{N}_e}{\partial \eta} \right\} \mathbf{J} = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \frac{\partial N_1}{\partial \eta} \\ \frac{\partial N_2}{\partial \xi} & \frac{\partial N_2}{\partial \eta} \\ \frac{\partial N_3}{\partial \xi} & \frac{\partial N_3}{\partial \eta} \\ \frac{\partial N_4}{\partial \xi} & \frac{\partial N_4}{\partial \eta} \end{bmatrix} \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} \quad (2.23)$$

$$B = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_1}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_1}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_1}{\partial \eta} \frac{\partial \eta}{\partial y} \\ \frac{\partial N_2}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_2}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_2}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_2}{\partial \eta} \frac{\partial \eta}{\partial y} \\ \frac{\partial N_3}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_3}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_3}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_3}{\partial \eta} \frac{\partial \eta}{\partial y} \\ \frac{\partial N_4}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial N_4}{\partial \eta} \frac{\partial \eta}{\partial x} & \frac{\partial N_4}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial N_4}{\partial \eta} \frac{\partial \eta}{\partial y} \end{bmatrix} = [4 \times 2] \quad (2.24)$$

In the following, we are going to evaluate first the shape functions N and then the geometric terms like $\partial \xi / \partial x$, etc.

Shape Functions and Their Derivatives Let us assume in the following a linear temperature field in parametric (ξ, η) -space

$$T_e(\xi, \eta) = a_1 + a_2 \xi + a_3 \eta + a_4 \xi \eta \quad (2.25)$$

or in vector notation

$$T_e(\xi, \eta) = \mathcal{X}^T \mathbf{a} = \begin{bmatrix} 1 & \xi & \eta & \xi \eta \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{Bmatrix} \quad (2.26)$$

Evaluating Eq. (2.26) for all four nodes of the quadrilateral element (Figure 2.5) gives

$$\text{node 1: } T_{e,1} = T(\xi = -1, \eta = -1) = a_1 - a_2 - a_3 + a_4 \quad (2.27)$$

$$\text{node 2: } T_{e,2} = T(\xi = 1, \eta = -1) = a_1 + a_2 - a_3 - a_4 \quad (2.28)$$

$$\text{node 3: } T_{e,3} = T(\xi = 1, \eta = 1) = a_1 + a_2 + a_3 + a_4 \quad (2.29)$$

$$\text{node 4: } T_{e,4} = T(\xi = -1, \eta = 1) = a_1 - a_2 + a_3 - a_4 \quad (2.30)$$

or in matrix notation

$$\begin{Bmatrix} T_{e,1} \\ T_{e,2} \\ T_{e,3} \\ T_{e,4} \end{Bmatrix} = \underbrace{\begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}}_{\mathbf{X}} \begin{Bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{Bmatrix} \quad (2.31)$$

Solving for $\mathbf{a}$ gives

$$\begin{Bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{Bmatrix} = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix} \begin{Bmatrix} T_{e,1} \\ T_{e,2} \\ T_{e,3} \\ T_{e,4} \end{Bmatrix} \quad (2.32)$$

or

$$\mathbf{a} = \mathbf{A} \mathbf{T}_{e,n} = \mathbf{X}^{-1} \mathbf{T}_{e,n} \quad (2.33)$$

The vector of shape functions results as

$$\mathbf{N}_e^T = \mathcal{X}^T \mathbf{A} = \{1 \quad \xi \quad \eta \quad \xi\eta\} \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix} = \{N_1 \quad N_2 \quad N_3 \quad N_4\} \quad (2.34)$$

or

$$N_1 = \frac{1}{4}(1 - \xi)(1 - \eta), \quad N_2 = \frac{1}{4}(1 + \xi)(1 - \eta) \quad (2.35)$$

$$N_3 = \frac{1}{4}(1 + \xi)(1 + \eta), \quad N_4 = \frac{1}{4}(1 - \xi)(1 + \eta) \quad (2.36)$$

One may note that each N_i ($i = 1, \dots, 4$) is unity when ξ and η assume coordinates of node i , but zero when ξ and η assume the coordinates of any other node. The graphical representation of the linear shape functions is shown in Figure 2.6.

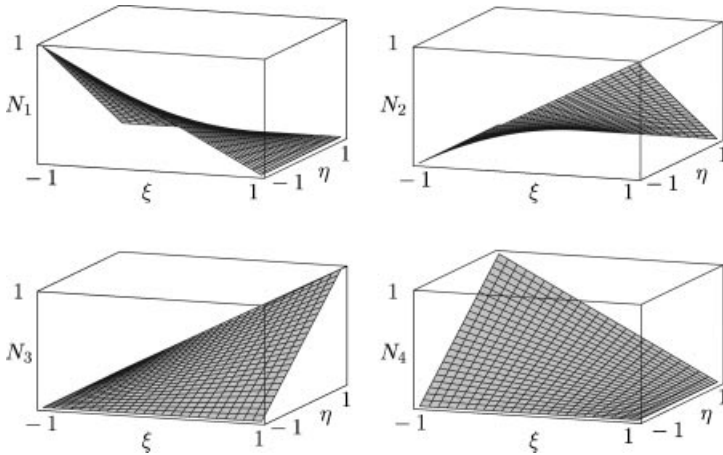


Figure 2.6 Linear shape functions for a plane element.

In a Cartesian x, y -coordinate system, the shape functions would be expressed for a rectangular element of dimension $a \times b$ (coordinate system in the element center and aligned to the edges) in the following way:

$$N_1(x, y) = \frac{1}{4ab} \cdot (a - x)(b - y), \quad N_2(x, y) = \frac{1}{4ab} \cdot (a + x)(b - y) \quad (2.37)$$

$$N_3(x, y) = \frac{1}{4ab} \cdot (a + x)(b + y), \quad N_4(x, y) = \frac{1}{4ab} \cdot (a - x)(b + y) \quad (2.38)$$

Introducing the variable substitution $x/a = \xi$ and $y/b = \eta$ gives the formulation in parametric space. The derivatives with respect to the parametric coordinates can easily be obtained as

$$\frac{\partial N_1}{\partial \xi} = \frac{1}{4}(-1 + \eta); \quad \frac{\partial N_1}{\partial \eta} = \frac{1}{4}(-1 + \xi) \quad (2.39)$$

$$\frac{\partial N_2}{\partial \xi} = \frac{1}{4}(+1 - \eta); \quad \frac{\partial N_2}{\partial \eta} = \frac{1}{4}(-1 - \xi) \quad (2.40)$$

$$\frac{\partial N_3}{\partial \xi} = \frac{1}{4}(+1 + \eta); \quad \frac{\partial N_3}{\partial \eta} = \frac{1}{4}(+1 + \xi) \quad (2.41)$$

$$\frac{\partial N_4}{\partial \xi} = \frac{1}{4}(-1 - \eta); \quad \frac{\partial N_4}{\partial \eta} = \frac{1}{4}(+1 - \xi) \quad (2.42)$$

Geometric Derivatives $\partial/\partial x$, etc. The geometric derivatives in Eq. (2.24), i.e. $\partial \xi / \partial x$, $\partial \xi / \partial y$, $\partial \eta / \partial x$, $\partial \eta / \partial y$, can be calculated based on

$$\begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} = \frac{1}{J} \cdot \begin{bmatrix} \frac{\partial y}{\partial \eta} & -\frac{\partial x}{\partial \eta} \\ -\frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \xi} \end{bmatrix} \quad (2.43)$$

where the Jacobian J is given by $J = \frac{\partial x \partial y}{\partial \xi \partial \eta} - \frac{\partial x \partial y}{\partial \eta \partial \xi}$. Let us assume the same interpolation for the global x and y coordinate as for the temperature:

$$x(\xi, \eta) = N_1(\xi, \eta) \cdot x_1 + N_2(\xi, \eta) \cdot x_2 + N_3(\xi, \eta) \cdot x_3 + N_4(\xi, \eta) \cdot x_4 \quad (2.44)$$

$$y(\xi, \eta) = N_1(\xi, \eta) \cdot y_1 + N_2(\xi, \eta) \cdot y_2 + N_3(\xi, \eta) \cdot y_3 + N_4(\xi, \eta) \cdot y_4 \quad (2.45)$$

Remark: the *global* coordinates of the nodes 1, ..., 4 can be used for $x_1, \dots, x_4$ and $y_1, \dots, y_4$. Thus, the derivatives can easily be obtained as

$$\frac{\partial x}{\partial \xi} = \frac{1}{4}((-1 + \eta)x_1 + (1 - \eta)x_2 + (1 + \eta)x_3 + (-1 - \eta)x_4) \quad (2.46)$$

$$\frac{\partial \gamma}{\partial \xi} = \frac{1}{4}((-1 + \eta)\gamma_1 + (1 - \eta)\gamma_2 + (1 + \eta)\gamma_3 + (-1 - \eta)\gamma_4) \quad (2.47)$$

$$\frac{\partial x}{\partial \eta} = \frac{1}{4}((-1 + \xi)x_1 + (-1 - \xi)x_2 + (1 + \xi)x_3 + (1 - \xi)x_4) \quad (2.48)$$

$$\frac{\partial \gamma}{\partial \eta} = \frac{1}{4}((-1 + \xi)\gamma_1 + (-1 - \xi)\gamma_2 + (1 + \xi)\gamma_3 + (1 - \xi)\gamma_4) \quad (2.49)$$

Remark: For a rectangle or a parallelogram, the derivatives are simple constants independent of ξ and η .

Based on the derived equations, the triple matrix product $\mathbf{B}\mathbf{k}\mathbf{B}^T$ can now be numerically calculated.

Numerical Integration Elementary integration formulas, such as the trapezoidal or Simpson rule, often assume equally spaced data and can become somewhat limited in accuracy and efficiency when used in finite element analysis. Gauss quadrature or integration has become the accepted numerical integration scheme in the majority of finite element applications. The Gauss–Legendre quadrature locates sampling points and assign weights so as to minimize integration error when the integrand is a general polynomial. Thus, for a given level of accuracy, Gauss quadrature uses fewer sampling points than other integration rules. Using Gauss–Legendre integration, one can write that

$$\int_{\Omega_e} f(x, z) d\Omega_e = \int_{\Omega'_e} f'(\xi, \eta) J d\Omega'_e = \int_{-1}^1 \int_{-1}^1 t \cdot f'(\xi, \eta) J d\xi d\eta = \sum_g t \cdot f'(\xi, \eta)_g J_g W_g \quad (2.50)$$

where $J = \frac{\partial x \partial y}{\partial \xi \partial \eta} - \frac{\partial x \partial \gamma}{\partial \eta \partial \xi}$, t is the thickness of the element, $(\xi, \eta)_g$ are the coordinates of the integration or Gauss points and W_g are the corresponding weighting factors. The locations of the integration points and values of associated weights are given elsewhere [71,72].

RHS of the Weak Statement The RHS of the weak statement (2.21) needs to be evaluated for each node along the element boundary Γ_e . For node 1, the shape function N_1 is equal to one and identically zero for all other nodes. In addition, all other shape functions are identically zero for node 1 (Figure 2.6). The expression $(\nabla T)^T \mathbf{n} = (\text{grad } T)^T \mathbf{n} = \partial T / \partial \mathbf{n}$ is equal to the projection of the gradient vector of the temperature in the direction of the boundary normal vector.

Since we have at each node two different normal vectors, one may calculate this expression for node 1 as (Figure 2.7):

$$k \left\{ \frac{\partial T}{\partial x} \frac{\partial T}{\partial y} \right\} \begin{Bmatrix} -1 \\ 0 \end{Bmatrix} + k \left\{ \frac{\partial T}{\partial x} \frac{\partial T}{\partial y} \right\} \begin{Bmatrix} 0 \\ -1 \end{Bmatrix} = \left(-k \frac{\partial T}{\partial x} - k \frac{\partial T}{\partial y} \right)_{\text{node 1}} \quad (2.51)$$

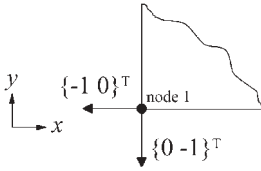


Figure 2.7 Normal vectors for RHS evaluation of Eq. (2.21) at node 1.

which is equal to the heat flux entering the element at node 1. Similar results can be obtained for all other nodes and the RHS of the weak statement can be written as

$$\int_{\Gamma_e} \mathbf{N}_e (k \nabla T)^T \mathbf{n} d\Gamma_e = \left\{ \begin{array}{l} \left(-k \frac{\partial T}{\partial x} - k \frac{\partial T}{\partial y} \right)_{\text{node 1}} \\ \left(k \frac{\partial T}{\partial x} - k \frac{\partial T}{\partial y} \right)_{\text{node 2}} \\ \left(+k \frac{\partial T}{\partial x} + k \frac{\partial T}{\partial y} \right)_{\text{node 3}} \\ \left(-k \frac{\partial T}{\partial x} + k \frac{\partial T}{\partial y} \right)_{\text{node 4}} \end{array} \right\} \quad (2.52)$$

From Eq. (2.52), we can see that only the magnitude and the sign of a heat flux can be applied at a node as a boundary condition (BC). However, a component in a specific coordinate direction (e.g. only a heat flux in the x -direction) cannot be applied since only the *sum* of all components (in the considered 2D case, i.e. in x - and y -direction) is applied at a node.

Example Let us inspect a distorted two-dimensional element (Figure 2.8) where the two nodal temperatures T_1 and T_2 are given as boundary conditions and the other two nodal temperatures are unknowns.

For this distorted element, the geometrical derivatives are

$$\frac{\partial \xi}{\partial x} = \frac{7/4 + 1/4\xi}{(7/4 + 1/4\eta)(7/4 + 1/4\xi) - (1/4 + 1/4\xi)(1/4 + 1/4\eta)} \quad (2.53)$$

$$\frac{\partial \xi}{\partial y} = -\frac{1/4 + 1/4\xi}{(7/4 + 1/4\eta)(7/4 + 1/4\xi) - (1/4 + 1/4\xi)(1/4 + 1/4\eta)} \quad (2.54)$$

$$\frac{\partial \eta}{\partial x} = -\frac{1/4 + 1/4\eta}{(7/4 + 1/4\eta)(7/4 + 1/4\xi) - (1/4 + 1/4\xi)(1/4 + 1/4\eta)} \quad (2.55)$$

$$\frac{\partial \eta}{\partial y} = \frac{7/4 + 1/4\eta}{(7/4 + 1/4\eta)(7/4 + 1/4\xi) - (1/4 + 1/4\xi)(1/4 + 1/4\eta)} \quad (2.56)$$

and the element conductivity matrix results as

$$K_e = \begin{bmatrix} 0.064835 & -0.021868 & -0.021099 & -0.021868 \\ -0.021868 & 0.084161 & -0.013121 & -0.049173 \\ -0.021099 & -0.013121 & 0.047340 & -0.013121 \\ -0.021868 & -0.049173 & -0.013121 & 0.084161 \end{bmatrix} \quad (2.57)$$

from which under consideration of the boundary conditions the nodal temperature vector can be obtained as

$$T_e = \{100 \quad 120 \quad 109.178295 \quad 113.116279\}^T \quad (2.58)$$

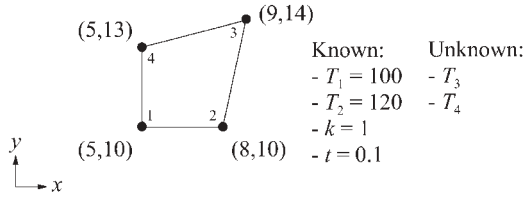


Figure 2.8 2D heat transfer problem with a distorted element.

2.2.4.1 General Rectangular Quad4 Element

In the following, the general element stiffness matrix for a rectangular Quad4 element of arbitrary dimensions a and b (Figure 2.9) will be derived under the following assumptions:

- constant thickness t ,
- constant thermal conductivity k ,
- orientation of the x - and y -axes parallel to the global COS,
- rectangular shape, all internal angles are equal to 90° .

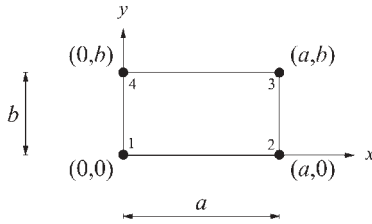


Figure 2.9 General rectangular Quad4 element.

The geometrical derivatives for this rectangular element are

$$\frac{\partial x}{\partial \eta} = 0, \frac{\partial y}{\partial \eta} = \frac{1}{2}b, \frac{\partial x}{\partial \xi} = \frac{1}{2}a, \frac{\partial y}{\partial \xi} = 0 \quad (2.59)$$

and

$$\frac{\partial \xi}{\partial x} = \frac{2}{a}, \frac{\partial \eta}{\partial x} = 0, \frac{\partial \xi}{\partial y} = 0, \frac{\partial \eta}{\partial y} = \frac{2}{b} \quad (2.60)$$

The temperature gradient matrix is given as

$$\mathbf{B} = \begin{bmatrix} \frac{-1+\eta}{2a} & \frac{-1+\xi}{2b} \\ -\frac{-1+\eta}{2a} & -\frac{-1+\xi}{2b} \\ \frac{1+\eta}{2a} & \frac{1+\xi}{2b} \\ -\frac{1+\eta}{2a} & -\frac{1+\xi}{2b} \end{bmatrix} = [4 \times 2] \quad (2.61)$$

and is transposed as

$$\mathbf{B}^T = \begin{bmatrix} \frac{-1+\eta}{2a} & -\frac{-1+\eta}{2a} & \frac{1+\eta}{2a} & -\frac{1+\eta}{2a} \\ \frac{-1+\xi}{2b} & -\frac{-1+\xi}{2b} & \frac{1+\xi}{2b} & -\frac{1+\xi}{2b} \end{bmatrix} = [2 \times 4] \quad (2.62)$$

Under consideration of a constant conductivity matrix (Eq. (2.3)), the triple matrix product $\mathbf{BkB}^T$ can be calculated as

$$\mathbf{BkB}^T = \frac{k}{4} \begin{bmatrix} \frac{(-1+\eta)^2}{a^2} + \frac{(-1+\xi)^2}{b^2} & -\frac{(1-\eta)^2}{a^2} + \frac{(1-\xi)^2}{b^2} & \frac{(\eta^2-1)}{a^2} + \frac{(\xi^2-1)}{b^2} & -\frac{(\eta^2-1)}{a^2} - \frac{(1-\xi)^2}{b^2} \\ -\frac{(1-\eta)^2}{a^2} + \frac{(1-\xi)^2}{b^2} & \frac{(1-\eta)^2}{a^2} + \frac{(1+\xi)^2}{b^2} & \frac{(1-\eta^2)}{a^2} - \frac{(1+\xi)^2}{b^2} & -\frac{(1-\eta^2)}{a^2} - \frac{(1-\xi^2)}{b^2} \\ \frac{(\eta^2-1)}{a^2} + \frac{(\xi^2-1)}{b^2} & -\frac{(1-\eta^2)}{a^2} + \frac{(1+\xi)^2}{b^2} & \frac{(1+\eta)^2}{a^2} + \frac{(1+\xi)^2}{b^2} & -\frac{(1+\eta)^2}{a^2} + \frac{(1-\xi^2)}{b^2} \\ -\frac{(\eta^2-1)}{a^2} - \frac{(1-\xi)^2}{b^2} & -\frac{(1-\eta^2)}{a^2} - \frac{(1-\xi^2)}{b^2} & -\frac{(1+\eta)^2}{a^2} + \frac{(1-\xi^2)}{b^2} & \frac{(1+\eta)^2}{a^2} + \frac{(1-\xi)^2}{b^2} \end{bmatrix} \quad (2.63)$$

To finally derive the element stiffness matrix, the triple matrix product needs to be numerically integrated. The Jacobian for the coordinate transformation to ξ - η -space is given by

$$J = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} = \frac{1}{4} \cdot ab \quad (2.64)$$

Case 1: One-Point Gauss Integration (Reduced Integration) In this case, the weighting factor is equal to $W_g = 4$ and the coordinate for the functional evaluation is $\xi_g = \eta_g = 0$. Thus, the integral becomes

$$\int_{\Omega'_e} \mathbf{BkB}^T d\Omega'_e = \mathbf{B}(\xi_g = 0, \eta_g = 0) \mathbf{kB}^T(\xi_g = 0, \eta_g = 0) \cdot J \cdot W_g \cdot t \quad (2.65)$$

which finally gives

$$\int_{\Omega'_e} \mathbf{B} \mathbf{k} \mathbf{B}^T d\Omega'_e = \frac{k}{4} \cdot \frac{t}{ab} \begin{bmatrix} a^2 + b^2 & a^2 - b^2 & -a^2 - b^2 & -a^2 + b^2 \\ a^2 - b^2 & a^2 + b^2 & -a^2 + b^2 & -a^2 - b^2 \\ -a^2 - b^2 & -a^2 + b^2 & a^2 + b^2 & a^2 - b^2 \\ -a^2 + b^2 & -a^2 - b^2 & a^2 - b^2 & a^2 + b^2 \end{bmatrix} \quad (2.66)$$

Numerical Example Let us examine a rectangular two-dimensional element (Figure 2.10) where two nodal temperatures are given as boundary conditions and the other two nodal temperatures are unknowns.

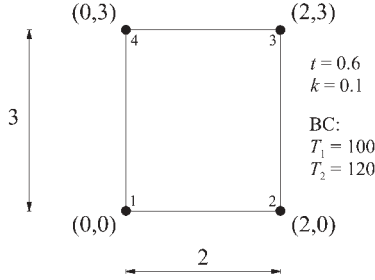


Figure 2.10 Rectangular Quad4 element, reduced integration.

The temperature gradient matrix and the element conductivity matrix can be calculated as

$$\mathbf{B} = \begin{bmatrix} -\frac{1}{4} & -\frac{1}{6} \\ \frac{1}{4} & \frac{1}{6} \\ \frac{1}{4} & -\frac{1}{6} \\ \frac{1}{4} & \frac{1}{6} \\ -\frac{1}{4} & \frac{1}{6} \\ -\frac{1}{4} & -\frac{1}{6} \end{bmatrix}; \quad \mathbf{K}_e = \frac{1}{4000} \begin{bmatrix} 13 & -5 & -13 & 5 \\ -5 & 13 & 5 & -13 \\ -13 & 5 & 13 & -5 \\ 5 & -13 & -5 & 13 \end{bmatrix} \quad (2.67)$$

Finally, the nodal temperature vector can be obtained as

$$\mathbf{T}_e = \{100 \quad 120 \quad 100 \quad 120\}^T \quad (2.68)$$

Note that in many commercial finite element codes, an *additional* variationally consistent conductivity term is included to eliminate the hourglass modes that are normally associated with reduced integration.

Case 2: Four-Point Gauss Integration (Full Integration) In this case, all weighting factors are equal to $W_g = 1$ and the coordinates for the functional evaluation are:

$$g_1 = \left(-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right), g_2 = \left(\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right), g_3 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right), g_4 = \left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right) \quad (2.69)$$

Thus, the integral becomes

$$\begin{aligned}
 \int_{\Omega'_e} \mathbf{B} \mathbf{k} \mathbf{B}^T d\Omega'_e &= \mathbf{B} \left(\xi_g = -\frac{1}{\sqrt{3}}, \eta_g = -\frac{1}{\sqrt{3}} \right) \mathbf{k} \mathbf{B}^T \left(\xi_g = -\frac{1}{\sqrt{3}}, \eta_g = -\frac{1}{\sqrt{3}} \right) \cdot J \cdot 1 \cdot t \\
 &+ \mathbf{B} \left(\xi_g = \frac{1}{\sqrt{3}}, \eta_g = -\frac{1}{\sqrt{3}} \right) \mathbf{k} \mathbf{B}^T \left(\xi_g = \frac{1}{\sqrt{3}}, \eta_g = -\frac{1}{\sqrt{3}} \right) \cdot J \cdot 1 \cdot t \\
 &+ \mathbf{B} \left(\xi_g = \frac{1}{\sqrt{3}}, \eta_g = \frac{1}{\sqrt{3}} \right) \mathbf{k} \mathbf{B}^T \left(\xi_g = \frac{1}{\sqrt{3}}, \eta_g = \frac{1}{\sqrt{3}} \right) \cdot J \cdot 1 \cdot t \\
 &+ \mathbf{B} \left(\xi_g = -\frac{1}{\sqrt{3}}, \eta_g = \frac{1}{\sqrt{3}} \right) \mathbf{k} \mathbf{B}^T \left(\xi_g = -\frac{1}{\sqrt{3}}, \eta_g = \frac{1}{\sqrt{3}} \right) \cdot J \cdot 1 \cdot t
 \end{aligned} \tag{2.70}$$

Evaluation of this sum gives

$$\int_{\Omega'_e} \mathbf{B} \mathbf{k} \mathbf{B}^T d\Omega'_e a = \frac{k}{3} \cdot \frac{t}{ab} \begin{bmatrix} a^2 + b^2 & \frac{1}{2}a^2 - b^2 & -\frac{1}{2}a^2 - \frac{1}{2}b^2 & -a^2 + \frac{1}{2}b^2 \\ \frac{1}{2}a^2 - b^2 & a^2 + b^2 & -a^2 + \frac{1}{2}b^2 & -\frac{1}{2}a^2 - \frac{1}{2}b^2 \\ -\frac{1}{2}a^2 - \frac{1}{2}b^2 & -a^2 + \frac{1}{2}b^2 & a^2 + b^2 & \frac{1}{2}a^2 - b^2 \\ -a^2 + \frac{1}{2}b^2 & -\frac{1}{2}a^2 - \frac{1}{2}b^2 & \frac{1}{2}a^2 - b^2 & a^2 + b^2 \end{bmatrix} \tag{2.71}$$

Numerical Example (see Figure 2.10) In the case of four-point Gauss integration, the element conductivity matrix results as

$$\mathbf{K}_e = \begin{bmatrix} 0.0433 & -0.0233 & -0.0217 & 0.0017 \\ -0.0233 & 0.0433 & 0.0017 & -0.0217 \\ -0.0217 & 0.0017 & 0.0433 & -0.0233 \\ 0.0017 & -0.0217 & -0.0233 & 0.0433 \end{bmatrix} \tag{2.72}$$

and the nodal temperature vector can be obtained as

$$\mathbf{T}_e = \{ 100 \quad 120 \quad 106.5 \quad 113.5 \}^T \tag{2.73}$$

which gives a difference smaller than 10% compared to the values given in Eq. (2.68).

2.2.4.2 Postprocessing

After the computation of the nodal temperature vector $\mathbf{T}_e = \{T_{e,1} T_{e,2} T_{e,3} T_{e,4}\}^T$ (cf. Eq. (2.73)), further quantities need to be calculated.

Temperature Gradients The temperature gradients are normally evaluated at the integration points in a postprocessing step after solving the system of equations.

Then these values at the integrations points are extrapolated to the element nodes in a graphical postprocessor. The temperature gradients are given in the considered 2D case in general as

$$\frac{\partial T_e}{\partial x} = \frac{\partial T_e(\xi, \eta)}{\partial \xi} \cdot \frac{\partial \xi}{\partial x} + \frac{\partial T_e(\xi, \eta)}{\partial \eta} \cdot \frac{\partial \eta}{\partial x}, \quad \frac{\partial T_e}{\partial y} = \frac{\partial T_e(\xi, \eta)}{\partial \xi} \cdot \frac{\partial \xi}{\partial y} + \frac{\partial T_e(\xi, \eta)}{\partial \eta} \cdot \frac{\partial \eta}{\partial y} \quad (2.74)$$

Based on the field approximation of the temperature, i.e. $T_e(\xi, \eta) = \sum N_i \cdot T_{e,i}$ ($i = 1, \dots, 4$), the derivatives of the temperature in ξ - η -space are simply obtained as

$$\frac{\partial T_e(\xi, \eta)}{\partial \xi} = \frac{\partial N_1}{\partial \xi} \cdot T_{e,1} + \frac{\partial N_2}{\partial \xi} \cdot T_{e,2} + \frac{\partial N_3}{\partial \xi} \cdot T_{e,3} + \frac{\partial N_4}{\partial \xi} \cdot T_{e,4} \quad (2.75)$$

$$\frac{\partial T_e(\xi, \eta)}{\partial \eta} = \frac{\partial N_1}{\partial \eta} \cdot T_{e,1} + \frac{\partial N_2}{\partial \eta} \cdot T_{e,2} + \frac{\partial N_3}{\partial \eta} \cdot T_{e,3} + \frac{\partial N_4}{\partial \eta} \cdot T_{e,4} \quad (2.76)$$

Based on these equations, the gradients in the x -direction are obtained for our example (four-point Gauss integration) at the integration points as

$$\left. \frac{\partial T_e}{\partial x} \right|_{g_1} = 7.147114, \left. \frac{\partial T_e}{\partial x} \right|_{g_2} = 7.147114, \left. \frac{\partial T_e}{\partial x} \right|_{g_3} = -0.647114, \left. \frac{\partial T_e}{\partial x} \right|_{g_4} = -0.647114 \quad (2.77)$$

and for the y -direction as

$$\left. \frac{\partial T_e}{\partial y} \right|_{g_1} = 2.598076, \left. \frac{\partial T_e}{\partial y} \right|_{g_2} = -2.598076, \left. \frac{\partial T_e}{\partial y} \right|_{g_3} = -2.598076, \left. \frac{\partial T_e}{\partial y} \right|_{g_4} = 2.598076 \quad (2.78)$$

Components of Heat Flux The components of the heat flux are also evaluated at the integration points. Taking the values of the temperature gradients and considering the general definition of the element heat flux vector, i.e. $\mathbf{q}_e = -k \nabla T_e$, the x -components of the heat flux vector result as

$$q_{e,x}^{g_1} = -0.714711, q_{e,x}^{g_2} = -0.714711, q_{e,x}^{g_3} = 0.064711, q_{e,x}^{g_4} = 0.064711 \quad (2.79)$$

while the y -components are gives as

$$q_{e,y}^{g_1} = -0.259808, q_{e,y}^{g_2} = 0.259808, q_{e,y}^{g_3} = 0.259808, q_{e,y}^{g_4} = -0.259808 \quad (2.80)$$

The total heat flux is obtained by vector addition, i.e. $q = \sqrt{q_x^2 + q_y^2}$, of the single components as

$$q_e^{g1} = 0.760469, q_e^{g2} = 0.760469, q_e^{g3} = 0.267745, q_e^{g4} = 0.267745 \quad (2.81)$$

Reaction Heat Flux The reaction heat flux is a nodal quantity and is obtained by multiplying the global stiffness matrix (without consideration of the BCs) with the global temperature result vector:

$$\mathbf{q}_r = \begin{bmatrix} 0.0433 & -0.0233 & -0.0217 & 0.0017 \\ -0.0233 & 0.0433 & 0.0017 & -0.0217 \\ -0.0217 & 0.0017 & 0.0433 & -0.0233 \\ 0.0017 & -0.0217 & -0.0233 & 0.0433 \end{bmatrix} \cdot \begin{Bmatrix} 100 \\ 120 \\ 106.5 \\ 113.5 \end{Bmatrix} = \begin{Bmatrix} -0.585 \\ 0.585 \\ 0 \\ 0 \end{Bmatrix} \quad (2.82)$$

2.2.5

Nonlinearities

In the following, a linear temperature dependency of the thermal conductivity in the form:

$$k(T) = k_0 + c \cdot T \quad (2.83)$$

is considered where k_0 and c take constant values. Let us assume additionally that the element is of rectangular shape (all internal angles equal to 90°) with arbitrary dimension a and b (Figure 2.9) parallel to the global x - and y -axes and constant thickness t . In order to introduce the expression for k in the element conductivity matrix of Eq. (2.18), its matrix notation in the form

$$\mathbf{k} = (k_0 + c \cdot T) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = (k_0 + c \cdot T) \mathbf{I} \quad (2.84)$$

must be used:

$$\int_{\Omega'_e} \mathbf{B} \mathbf{k} \mathbf{B}^T d\Omega'_e = \int_{\Omega'_e} \mathbf{B} (k_0 + c \cdot T) \mathbf{I} \mathbf{B}^T d\Omega'_e = \int_{\Omega'_e} \mathbf{B} k_0 \mathbf{I} \mathbf{B}^T d\Omega'_e + \int_{\Omega'_e} \mathbf{B} c T \mathbf{I} \mathbf{B}^T d\Omega'_e \quad (2.85)$$

$$= \int_{\Omega'_e} \mathbf{B} k_0 \mathbf{I} \mathbf{B}^T d\Omega'_e + \int_{\Omega'_e} \mathbf{B} c N_e^T T_e \mathbf{I} \mathbf{B}^T d\Omega'_e \quad (2.86)$$

Let us first examine the expression $N_e^T T_e \mathbf{I}$:

$$N_e^T T_e \mathbf{I} = \{ N_1 \quad N_2 \quad N_3 \quad N_4 \} \cdot \left\{ \begin{matrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{matrix} \right\} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (2.87)$$

$$= \begin{bmatrix} N_1 T_1 + N_2 T_2 + N_3 T_3 + N_4 T_4 & 0 \\ 0 & N_1 T_1 + N_2 T_2 + N_3 T_3 + N_4 T_4 \end{bmatrix} \quad (2.88)$$

$$= \begin{bmatrix} p & 0 \\ 0 & p \end{bmatrix} = \mathbf{p} = p \mathbf{I} \quad (2.89)$$

where the shape functions $N_1 - N_4$ are given by Eqs. (2.37) and (2.38). Now, the second expression of Eq. (2.86) can be written as

$$\int_{\Omega'_e} B c N_e^T T_e \mathbf{I} B^T d\Omega'_e = c \int_{\Omega'_e} B p \mathbf{I} B^T d\Omega'_e = c \int_{\Omega'_e} p B B^T d\Omega'_e a \quad (2.90)$$

where the function $p = p(\xi, \eta)$ is given by

$$p = \frac{1}{4} \cdot (1 - \xi)(1 - \eta) T_1 + \frac{1}{4} \cdot (1 + \xi)(1 - \eta) T_2 \\ + \frac{1}{4} \cdot (1 + \xi)(1 + \eta) T_3 + \frac{1}{4} \cdot (1 - \xi)(1 + \eta) T_4 \quad (2.91)$$

Using a four-point Gauss integration (full integration), the contribution to the conductivity matrix due to a linear T -proportional dependency of the conductivity is given as

$$K_{e,k-T} = \begin{bmatrix} K_{11} & K_{12} & K_{13} & K_{14} \\ K_{21} & K_{22} & K_{23} & K_{24} \\ K_{31} & K_{32} & K_{33} & K_{34} \\ K_{41} & K_{42} & K_{43} & K_{44} \end{bmatrix}_{e,k-T} \quad (2.92)$$

where the elements K_{ij} are given by

$$K_{11} = \frac{ct}{24ab} (a^2(3T_1 + T_2 + T_3 + 3T_4) + b^2(3T_1 + 3T_2 + T_3 + T_4)) \quad (2.93)$$

$$K_{12} = \frac{ct}{24ab} (a^2(T_1 + T_2 + T_3 + T_4) + b^2(-3T_1 - 3T_2 - T_3 - T_4)) = K_{21} \quad (2.94)$$

$$K_{13} = \frac{ct}{24ab} (-(a^2 + b^2) \cdot (T_1 + T_2 + T_3 + T_4)) = K_{31} \quad (2.95)$$

etc. The total element stiffness matrix results as the sum of Eqs. (2.71) and (2.92).

Numerical Example In the following example (Figure 2.11), a rectangular and a quadratic Quad4 element is investigated for different values of c (see Eq. (2.83)) which weights the temperature dependency of the conductivity. Additionally, different ranges of the given boundary conditions T_1 and T_2 are considered.

It can be seen from Table 2.1 that the major difference compared to the constant conductivity results stems from the difference in the temperature of the applied boundary conditions. The influence of the geometry and the weighting factor c is much smaller under the chosen model parameters.

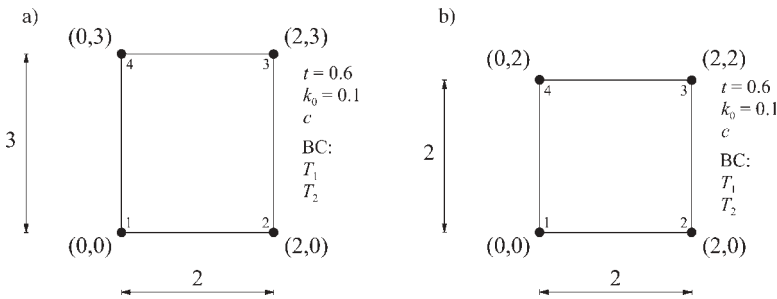


Figure 2.11 Rectangular Quad4 elements.

Table 2.1 Results for the Quad4 element with $k = k(T)$ -conductivity (the deviation refers to the result with constant conductivity, i.e. $c = 0$).

BC					Results		Deviation (%)	
a	b	c	T_1	T_2	T_3	T_4	3	4
2	3	0	100	120	106.500	113.500	—	—
		0.001	100	120	106.570	113.569	0.066	0.061
		0.1	100	120	106.632	113.631	0.124	0.115
		0	100	600	262.500	437.500	—	—
		0.001	100	600	282.899	456.910	7.771	4.437
		0.1	100	600	288.488	461.916	9.900	5.581
2	2	0	100	120	108.000	112.000	—	—
		0.001	100	120	108.076	112.076	0.070	0.068
		0	100	600	300.000	400.000	—	—
		0.001	100	600	321.219	422.147	7.073	5.537
		0.1	100	600	326.652	428.121	8.884	7.030

2.3

Modelling of Hollow-Sphere Structures

2.3.1

Geometry, Mesh and Boundary Conditions

The analysis of the macroscopic thermal conductivity of MHSS is performed by means of a finite element approach. The finite element model of the microstructure is exemplified in Figure 2.12, where the light gray elements correspond to the metallic sphere, whereas the dark gray elements are related to the joint. Depending on the considered joining technology, the joint represents the sintered neck or the adhesive connection between two neighboring spheres.

At the left and right side of the joints, two constant temperatures T_1 and T_2 are prescribed on parallel surfaces. The nodal reaction heat flux in the direction perpendicular to these surfaces is denoted as $\dot{Q}_j$. The total heat flux through one of the surfaces where the temperature boundary condition is prescribed is given by the sum of the single nodal reaction fluxes:

$$\dot{Q}(T_1, T_2) = \sum_j \dot{Q}_j(T_1, T_2) \quad (2.96)$$

where j denotes the number of nodes where the temperature T_1 or T_2 is assigned. The heat flux perpendicular to all remaining surfaces is zero which corresponds to periodic boundary conditions. It is shown in Refs. [73,74] that the influence of thermal radiation on the effective thermal conductivity of porous metals, especially at temperatures below 700 K is low and is therefore disregarded within this study. Furthermore, the open porosity of MHSS is small (partially bonded) or nonexistent (syntactic) and consequently also the effect of convection is excluded from the

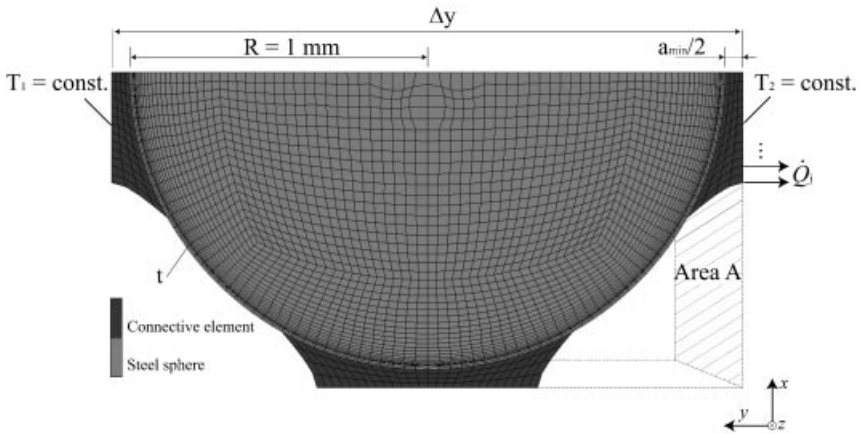


Figure 2.12 Finite element model incorporating boundary conditions.

numerical simulation. Due to these simplifications, Fourier's law yields the effective thermal conductivity $k(T_1, T_2)$ of the structure:

$$k(T_1, T_2) = \frac{\dot{Q}(T_1, T_2)}{A} \cdot \frac{\Delta y}{\Delta T} \quad (2.97)$$

The spatial distance Δy and the projected area A are defined by the geometry (Figure 2.12), the temperature difference $\Delta T = T_2 - T_1$ is given by the boundary conditions and the total heat flux $\dot{Q}(T_1, T_2)$ is the result of the finite element calculation.

Corresponding to measurements on real specimens (Figure 2.13), the outer diameter R of the hollow spheres is 1 mm, the sphere wall thickness t varies between 0.02 and 0.1 mm and the minimum distance between two neighboring spheres $a_{\min}$ is 0.12 mm for the cubic primitive topology. Furthermore, a second set of finite element models with syntactic morphology and different topologies (Figure 2.14) is generated, where the minimum distance $a_{\min}$ is 0.24 mm.

All geometries exhibit cubic symmetries and, by defining symmetric boundary conditions, only one-fourth (Figure 2.12) of a unit cell needs to be modelled.

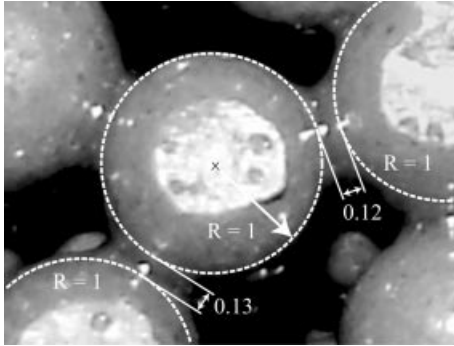


Figure 2.13 Geometric dimensions of a partially bonded MHSS.

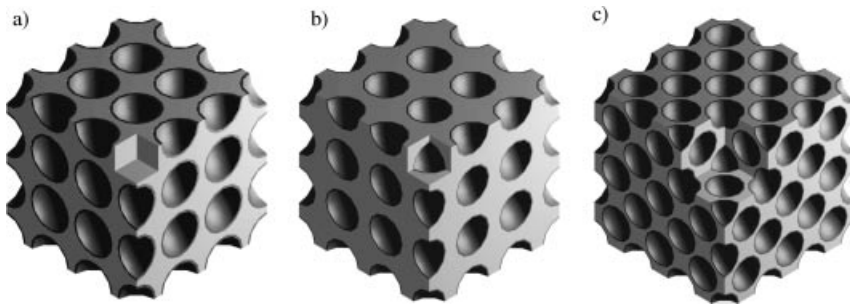


Figure 2.14 Topologies of syntactic hollow-sphere structures:
(a) primitive cubic; (b) body-centered cubic; (c) face-centered cubic.

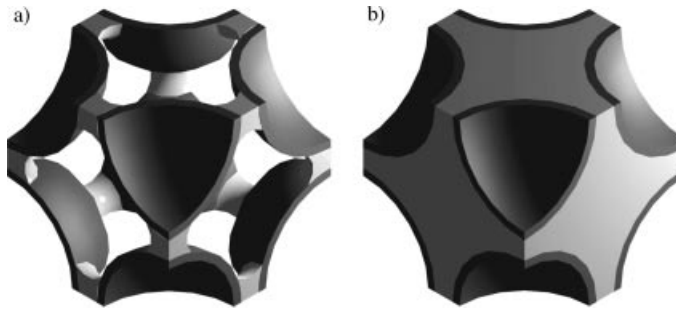


Figure 2.15 Morphologies of cubic primitive hollow sphere structures: (a) partially bonded; (b) syntactic.

Furthermore, two different morphologies, i.e. partially bonded or syntactic, are investigated for a cubic primitive topology (Figure 2.15).

In a second approach of the finite element analysis, the results of the thermal conductivities of the microstructure (unit cell) at low temperature gradients are assigned to a homogenized finite element model. Therefore, a simple mesh is assembled by planar rectangular elements (thickness 1) with the thermal conductivity corresponding to the results obtained for the microstructure of a primitive cubic MHSS. This procedure allows for the simulation of large structures without the necessity of modeling the whole microstructure. Finally, two aluminum face sheets are attached to the homogenized finite element model of the core in order to generate a sandwich structure with a varying face sheet thickness t . The evaluation of the directional thermal conductivity perpendicular to the face sheets of the sandwich structure is performed according to Eq. (2.97).

2.3.2

Material Properties

Two different types of material models are considered. First, temperature-independent properties are considered. The values of the average thermal conductivities and densities of these materials are listed in Table 2.2 [75].

In a second step, temperature-dependent material properties for nonlinear thermal analyses are incorporated in some of the calculation models. In Figures 2.16 and 2.17, the effective thermal conductivities k of these base materials are plotted versus the absolute temperature T .

Table 2.2 Material properties of MHSS constituents.

Material	Abbreviation	Thermal conductivity, k ($\text{W mm}^{-1} \text{K}^{-1}$)	Density ρ (g cm^{-3})
Steel	St	0.05000	7.9
Epoxy resin	Ep	0.00036	1.2

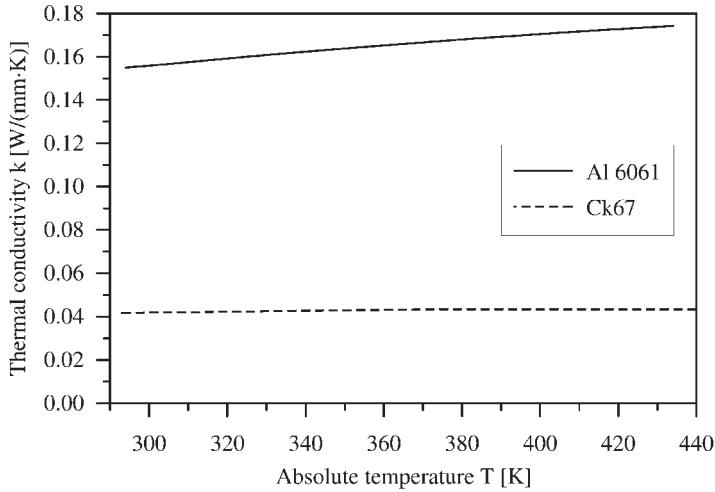


Figure 2.16 Temperature-dependent thermal conductivities of the metallic base materials Al 6061 (UNS A96061) [76] and Ck67 [77].

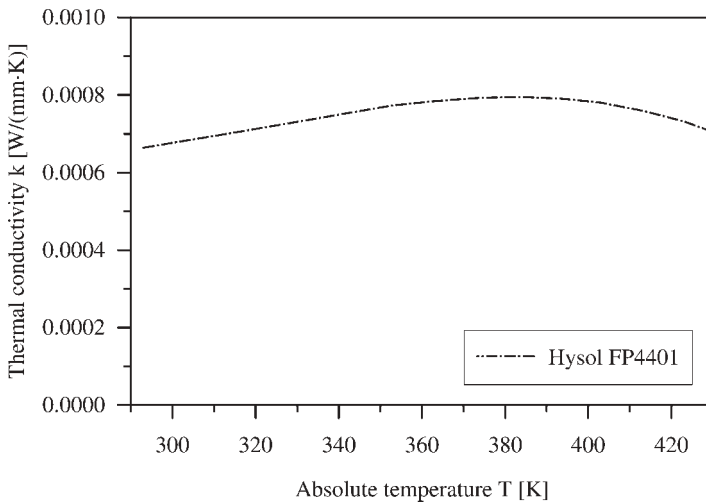


Figure 2.17 Temperature-dependent thermal conductivities of an epoxy resin [78].

2.4

Determination of the Effective Thermal Conductivities

In the following, the results of the finite element analysis for the effective thermal conductivities will be discussed. The influence of the joining technique, morphology, topology and temperature-dependent material properties will be analyzed.

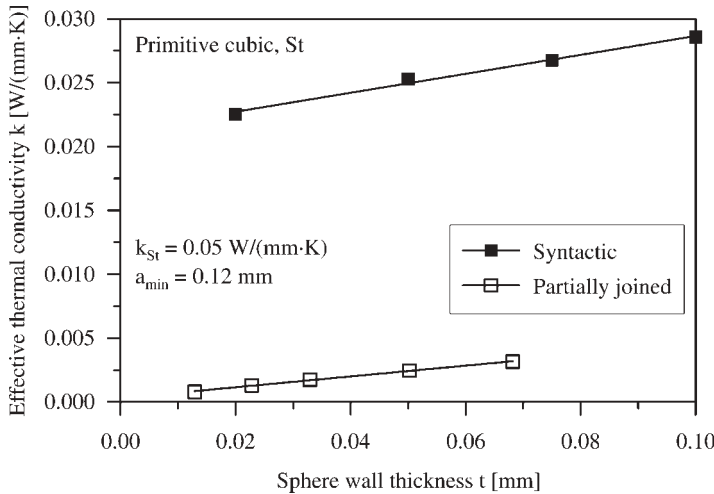


Figure 2.18 Influence of the morphology of *homogeneous* steel MHSS on the effective thermal conductivity.

2.4.1

Influence of the Morphology and Joining Technique

In the scope of the investigation of the influence of the morphology and the joining technique on the effective thermal properties of MHSS, only primitive cubic arrangements of the spheres are considered. Depending on the applied joining technique, different morphologies and material combinations are generated. Sintering yields a homogeneous and partially joined structure, whereas adhesive joining results in a heterogeneous (metal/epoxy) structure with varying morphology. Finally, a homogeneous syntactic structure can be achieved by applying casting technologies.

Figure 2.18 shows the influence of different morphologies for *homogeneous* steel structures. The effective thermal conductivity is plotted versus the sphere wall thickness t . As a result of the higher volume fraction of the matrix, the syntactic MHSS exhibit significant higher thermal conductivity. In contrast to this behavior, the partially bonded structures show only low values, especially for a small sphere wall thickness t .

In Figure 2.19, the influence of the morphology on the thermal properties of *adhesively* bonded structures is visualized. Due to the higher volume fraction of the matrix, the thermal conductivity of syntactic MHSS exceeds the values of the partial morphology. However, the deviation is smaller in comparison to the homogeneous structures. This phenomenon can be explained by the low thermal conductivity of the adhesive matrix. Increase of the volume fraction of the matrix therefore only slightly increases the effective conductivity of the structure.

Next, two different joining techniques for partially bonded MHSS are compared. Figure 2.20 shows the results obtained for a sintered and an adhesively bonded

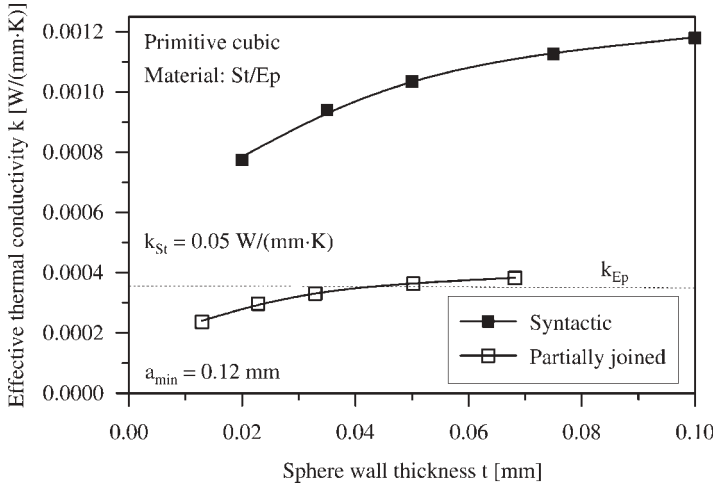


Figure 2.19 Influence of the morphology of *heterogeneous* MHSS on the effective thermal conductivity.

structure depending on the sphere wall thickness t . The effective thermal conductivities k of sintered structures are higher compared to the adhesively bonded MHSS and linearly increase with the thickness t . The low thermal conductivity of adhesively bonded structures lies within the range of the thermal conductivity of the adhesive.

The comparison of syntactic MHSS exhibiting different material combinations (Figure 2.21) yields large deviations. The explanation is the high volume fraction of the matrix for syntactic morphology in combination with the strongly different

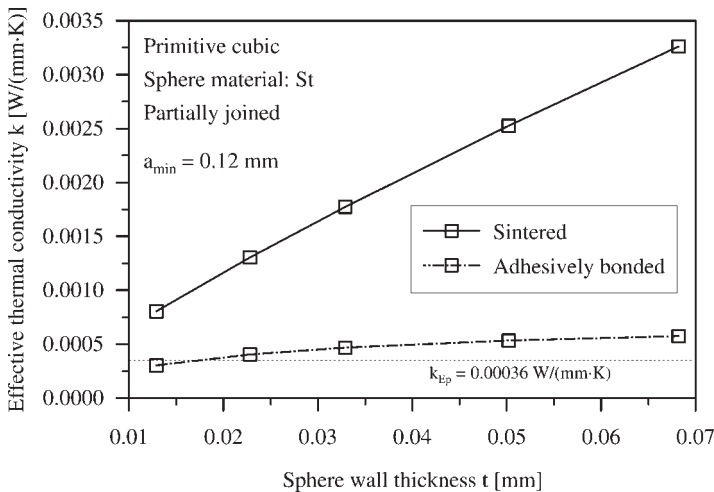


Figure 2.20 Influence of the joining technique of partially bonded MHSS on the effective thermal conductivity.

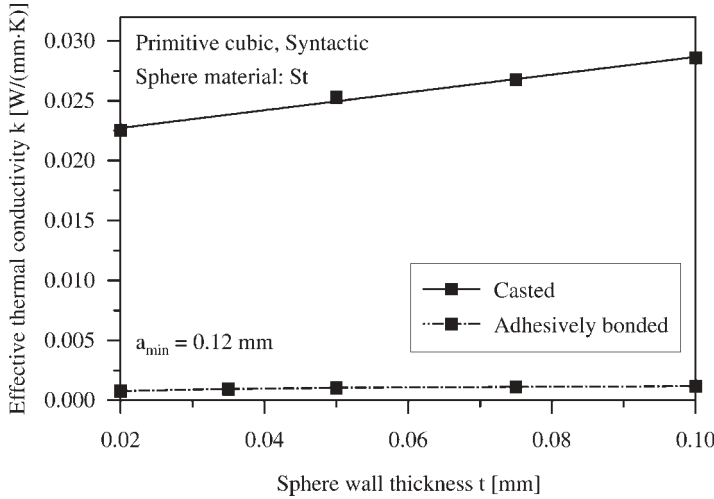


Figure 2.21 Influence of the joining technique of syntactic MHSS on the effective thermal conductivity.

thermal conductivities of the steel and epoxy resin base materials (Table 2.2). Therefore, the cast structure exhibits a much higher thermal conductivity than the adhesively bonded MHSS.

2.4.2

Influence of the Topology

Three different topologies, namely primitive cubic (■), body-centered cubic (●) and face-centered cubic (◆) arrangements of spheres (Figure 2.14), are considered. All analyses are performed for a syntactic morphology and two different material combinations (St and St/Ep) are investigated.

Figure 2.22 shows the results obtained for *homogeneous* steel structures. For all topologies, a linear characteristic of the effective thermal conductivity k in dependence on the sphere wall thickness t can be observed. The primitive cubic structures exhibit the maximum thermal conductivity k for a particular shell thickness t . However, by plotting the thermal conductivities versus the free volume V_i/V_u , a different picture arises. The free volume is equal to the volume of the spherical inclusion V_i divided by the volume of the unit cell V_u .

It can be seen in Figure 2.23 that all values can be approximated by a single straight line. Therefore, the thermal conductivity of homogeneous syntactic MHSS can be described only in dependence on the free volume. A linear fit based on the numerical data yields

$$k(V_i/V_u) = [-0.0581 \cdot (V_i/V_u) + 0.0479] \cdot \frac{W}{\text{mm} \cdot k} \quad (2.98)$$

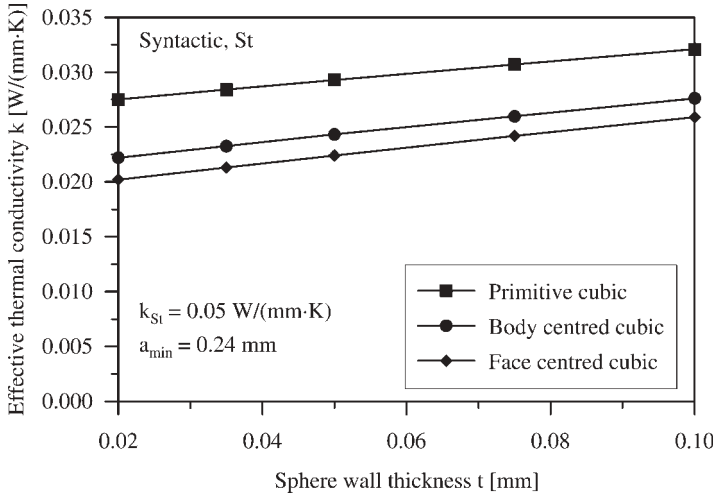


Figure 2.22 Influence of the topology on the thermal conductivity of *homogeneous* steel MHSS.

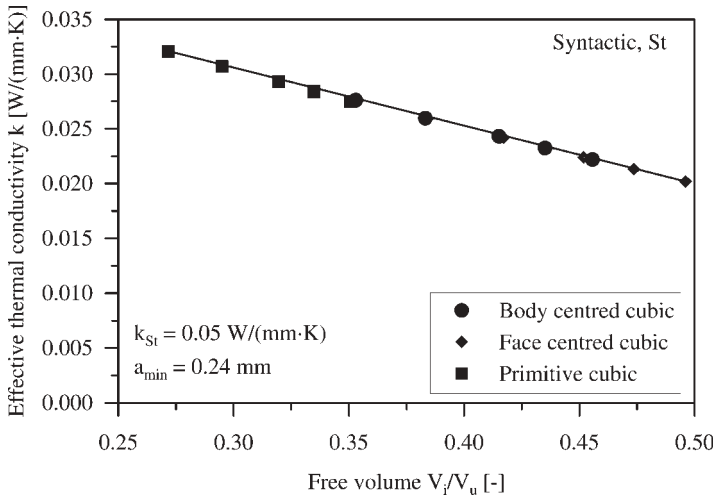


Figure 2.23 Thermal conductivity of *homogeneous* steel MHSS plotted versus the free volume.

or with the thermal conductivities k_b of an arbitrary base material

$$k(V_i/V_u) = [-1.162 \cdot (V_i/V_u) + 0.958] \cdot k_b \quad (2.99)$$

Figure 2.24 shows the thermal conductivities of *adhesively bonded* syntactic MHSS. Although the thermal conductivity increases with increasing sphere wall thickness, the gradient of the curve continuously decreases. The explanation is the high thermal

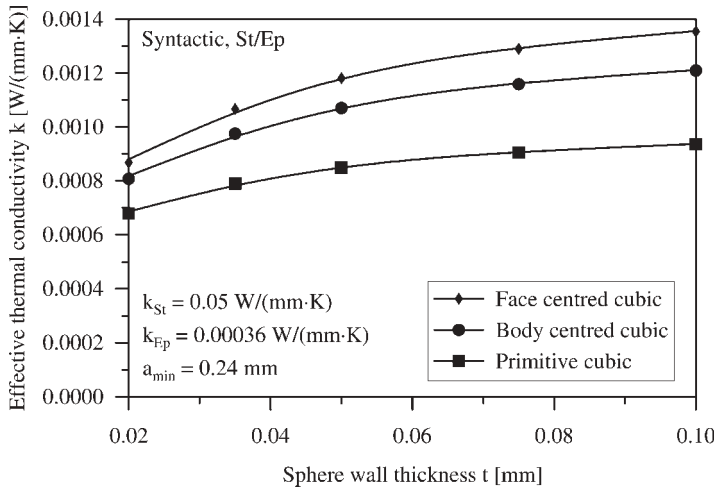


Figure 2.24 Influence of the topology on the thermal conductivity of heterogeneous MHSS.

resistance of the adhesive matrix between neighboring spheres. Enhancement of the volume fraction of the high thermal conducting sphere wall material therefore only slightly increases the overall thermal conductivity of the structure.

Analogous to the homogeneous structures, k is plotted versus the free volume V_i/V_u in Figure 2.25. It can be observed that the face-centered cubic arrangement of spheres yields maximum thermal conductivity for a particular value of the free volume. The explanation is the cubic densest packing of this topology which causes

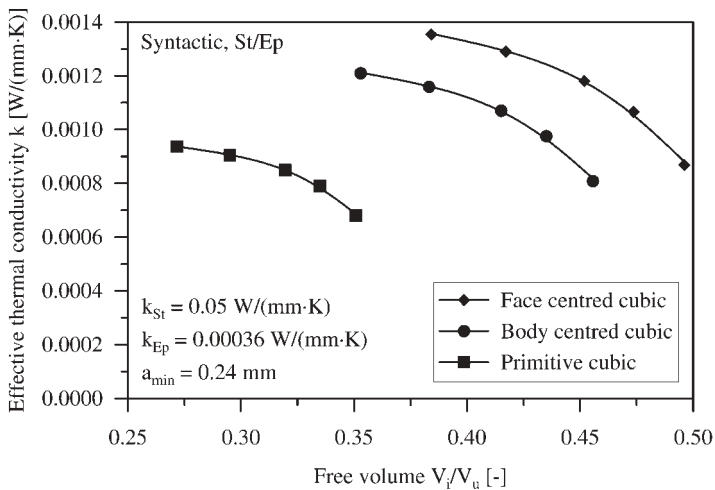


Figure 2.25 The dependence of the thermal conductivity of heterogeneous MHSS on the free volume.

the highest volume fraction (total volume of the metallic shell divided by the volume of the unit cell) of the metallic sphere wall material. The high thermal conductivity of the metal increases the effective thermal conductivity of the structure. Consequently, the primitive cubic topology which exhibits the lowest volume fraction of the metallic sphere wall material shows the minimum thermal conductivity.

2.4.3

Temperature-Dependent Material Properties

The determination of the effective thermal conductivity of MHSS incorporating temperature-dependent material properties requires the distinction of two different cases. First, a low temperature gradient where the temperature is approximately constant within the entire unit cell and, second, a high temperature gradient, where the changing temperature dependence of the base materials of the structure inside a single unit cell has to be accounted for.

2.4.3.1 Low Temperature Gradient

In the case of a low temperature gradient, the temperature inside the entire unit cell can be regarded as approximately constant. Therefore, the thermal conductivity of the MHSS can be determined only in dependence on this temperature. The temperature boundary conditions (Figure 2.12) are $T_1 = T_i + 0.01$ K and $T_2 = T_i - 0.01$ K for $T_i = 293, 303, \dots, 433$ K and the results of these calculations are summarized in Figures 2.26 and 2.27.

Figure 2.27 shows the temperature dependence of the thermal conductivity of adhesively bonded MHSS. In comparison to the results of sintered structures

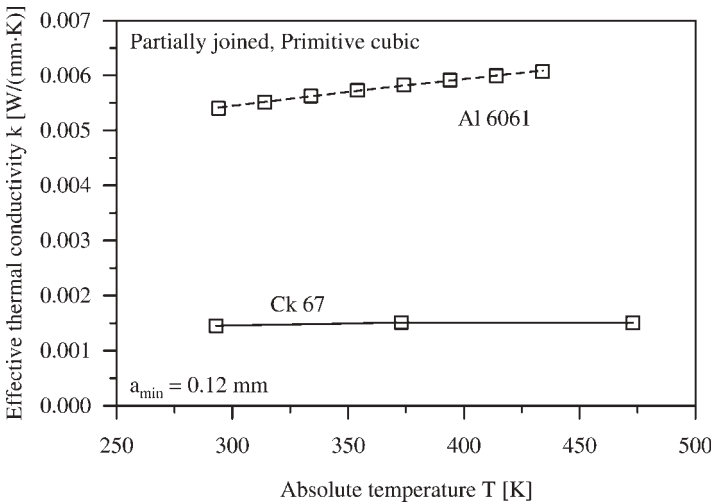


Figure 2.26 Effective thermal conductivity of sintered MHSS incorporating temperature-dependent base material parameters for low temperature gradients.

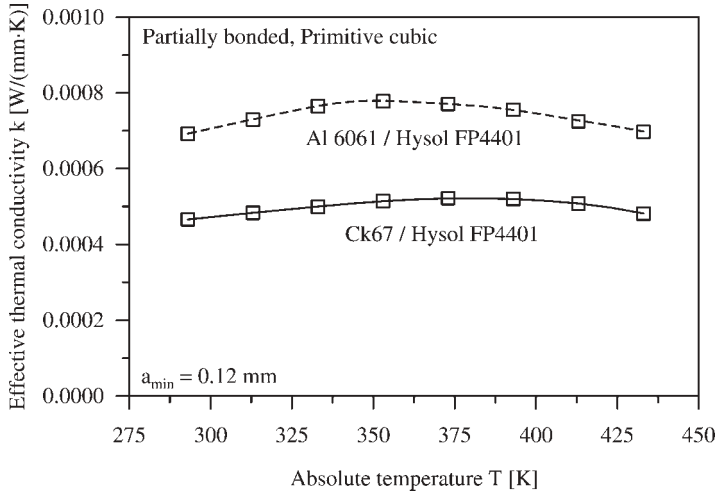


Figure 2.27 Effective thermal conductivity of adhesively bonded MHSS incorporating temperature-dependent base material parameters for low temperature gradients.

(Figure 2.26), the values of adhesively bonded MHSS are lower. The adhesively bonded structures exhibit a maximum of the conductivity at approximately 340 K (Al/Hysol) and 390 K (Ck67/Hysol). The conductivity of the sintered structures rises linearly with the absolute temperature within the designated range. The high thermal conductivity of the aluminum alloy (Figure 2.16) also increases the thermal conductivity of MHSS. In comparison, the utilization of CK67 as a sphere wall material decreases the thermal conductivity of the structure.

2.4.3.2 High Temperature Gradient

In contrast to the simplification in the previous section, high temperature gradients require the consideration of the temperature distribution inside the unit cell. Due to the temperature dependence of the thermal conductivities of the base materials (see Figures 2.16 and 2.17), the thermal conductivity of the unit cell depends on the absolute values of both temperatures T_1 and T_2 and cannot therefore be determined for particular temperatures. In order to confine the complexity of this investigation, the temperature T_1 is fixed at the constant temperature 298 K (approximately room temperature) and only the temperature T_2 is varied as 323, 348, 423 K (glass transition temperature 433 K [79] of the exopy resin being considered). The results are obtained for the unit cell as well as for a homogenized model of the MHSS. The homogenized model is assembled by planar rectangular elements and exhibits the thermal properties obtained in the previous section for the MHSS and low temperature gradients.

Figure 2.28 shows the results of both analyses. In the case of low temperature gradients (e.g. $T_2 = 323 \text{ K} \rightarrow \Delta T / \Delta y = 25 \text{ K} / 2.12 \text{ mm}$) the results obtained for both models almost coincide. However, also for the maximum temperature difference of 125 K the deviation reaches only 0.93%.

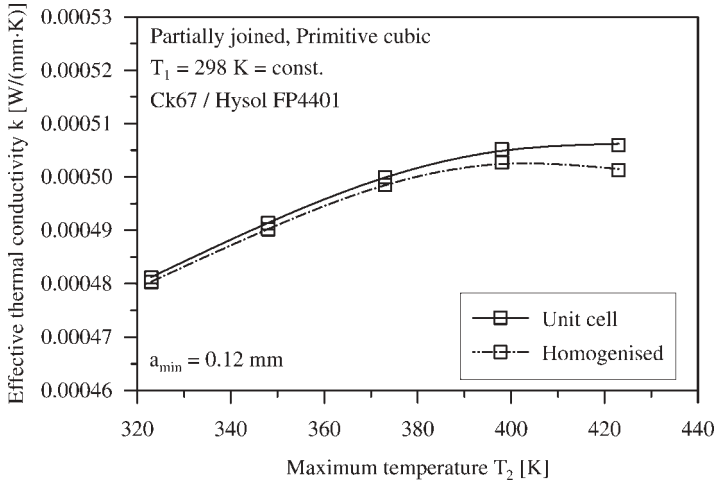


Figure 2.28 Effective thermal conductivity incorporating temperature dependent base material parameters for high temperature gradients.

2.4.4

Application Example: Sandwich Structure

In the following, sandwich panels with MHSS cores acting as a thermal insulating layer are considered. The effective thermal conductivity is determined in the direction of the normal vector of the face sheets. The temperatures prescribed at the upper and lower surfaces are 293 K and 433 K, respectively. The microstructure of the MHSS is homogenized and therefore represented by plane rectangular elements (2D approach) in order to reduce the required calculation time. As shown in the previous section, the deviation introduced by this simplification is small. Figure 2.29 summarizes the results of this investigation. The effective thermal conductivity is plotted versus the normalized face sheet thickness. This ratio is equal to the varying thickness f of the face sheets divided by the constant total height $h = 30$ mm of the structure and is defined for values between 0 (pure core material) and 0.5 (no core material, face sheets merge).

The thermal conductivity of the sandwich structure increases with increasing relative thickness of the face sheets. This phenomenon can be explained with the high thermal conductivity of aluminum alloy (Figure 2.16) in comparison to the insulating MHSS core material. Even in the case of very thin insulating layers ($f/h = 0.4$) the thermal conductivity of the sandwich panel only reaches approximately 1.5% of the values of the face sheet material. However, for further decrease of the thickness of the core, the thermal conductivity of the structure grows exponentially. In the following simulation, the thin adhesive layers which join the face sheets and core material are incorporated in the numerical simulation. The overall height h of the structure is 30 mm and the face sheet thickness t is 1 mm. Two different adhesive interface layers with a thickness t_{Adh} of 0.25 and 0.5 mm are considered. These interface layers exhibit the thermal properties of Hysol FP4401 (Figure 2.17) which

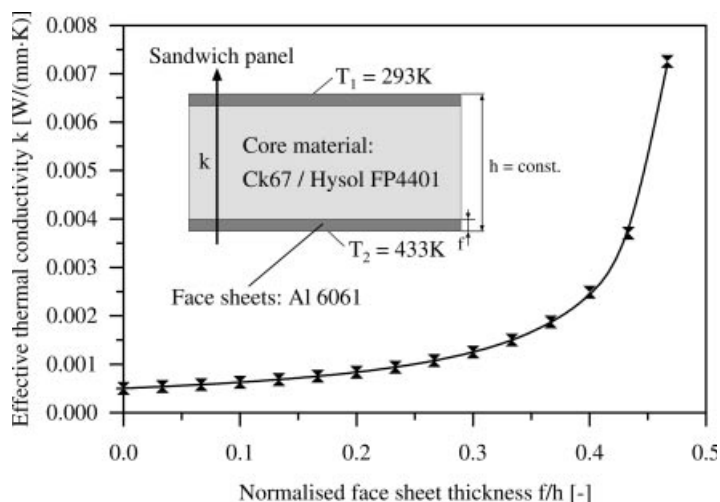


Figure 2.29 The dependence of the thermal conductivity of sandwich panels with MHSS cores on the normalized face sheet thickness.

are multiplied by a scale factor $s = 0.8, 1.0, 1.2$ in order to account for a change of the material properties due to chemical reactions. The findings are shown in Table 2.3.

It can be seen that the influence of the thin interface layer on the overall thermal conductivity is low. This result can be explained by the similar thermal conductivities of the adhesively bonded hollow-sphere structure (Figure 2.27) and the adhesive (Figure 2.17). Changing material properties of the adhesive layer ($\pm 20\%$), e.g. due to chemical reactions, results only in a very small influence on the macroscopic properties of the entire sandwich structure. The influence slightly increases with growing thickness t_{Adh} of the adhesive interface layer.

Table 2.3 Thermal conductivities in $\text{W mm}^{-1} \text{K}^{-1}$ of sandwich structures ($t = 2 \text{ mm}$) with thin adhesive interface layers.

Scale factor s	0.8	1.0	1.2
$t_{\text{Adh}} = 0.25 \text{ mm}$	0.582	0.584	0.585
$t_{\text{Adh}} = 0.50 \text{ mm}$	0.583	0.587	0.590
Without		0.581	

2.5 Conclusions

In the scope of this chapter, the effective thermal conductivity of metallic hollow-sphere structures was investigated. It was found that partial morphology exhibits lower thermal conductivity in comparison to syntactic structures. This result is valid for homogenous (sintered, casted) as well as heterogeneous (adhesively bonded)

structures. Furthermore, the influence of the topology on the thermal conductivity of MHSS was analyzed. A linear relation in dependence on the free volume was found to describe the thermal conductivity of homogeneous MHSS. In the case of adhesively bonded hollow-sphere structures, the face-centered cubic arrangement of the spheres yields the maximum thermal conductivity at a particular free volume. This can be explained by the most dense packing of the spheres for this topology and therefore the highest volume fraction of the metallic shells which exhibit a high thermal conductivity.

In the next step, temperature-dependent material properties were incorporated. Therefore, a primitive cubic topology with partial morphology was investigated. Two cases, namely a high and a low temperature gradient, were distinguished. In the case of low temperature gradients, the temperature in the structure was assumed to be approximately constant and temperature-dependent conductivities could be derived. For high temperature gradients, the thermal conductivities were obtained for room temperature at one and a variable temperature at the other side of the MHSS.

As an application example, a sandwich structure containing an adhesively bonded MHSS core with a partial morphology, was considered. It was found that the thermal conductivity of the sandwich is significantly lower compared to the conductivity of the face sheets, even for relatively thin cores.

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3

Thermal Properties of Composite Materials and Porous Media: Lattice-Based Monte Carlo Approaches

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3.1

Introduction

Ever since its development during World War II as part of the Manhattan Project, the Monte Carlo method has enjoyed countless applications in science and engineering. Inherently a computationally very demanding method, the Monte Carlo method has naturally become far more popular as computers have become faster, cheaper and more accessible. In transient thermal conduction problems, the Monte Carlo method using continuous random walks has been commonly used for many years to determine temperature profiles where there are arbitrarily shaped boundaries with arbitrarily varying boundary conditions (see, for example, [1]). Quite recently, a lattice-based Monte Carlo method, which is basically a type of simulation finite-difference method, has been developed to determine the effective thermal conductivity in some very simple models of two- and three-component composites and also simple models of porous media. In Section 3.2 of this chapter we describe such calculations in detail. The Monte Carlo method also has the potential to be used to provide temperature profiles in composite/porous media models too. This area is yet to be developed. In Section 3.3 we describe some recent preliminary calculations by the present authors.

3.2

Monte Carlo Methods of Calculation of the Effective Thermal Conductivity

In this section, we review Monte Carlo methods that have been developed to calculate the effective thermal conductivity in some simple models of composite materials and porous media. In Section 3.2.1, we show how the Einstein equation for Brownian motion is very useful for calculating the effective thermal diffusivity (conductivity). In Section 3.2.2 we show how Fick's first law (the Fourier equation) can also be used for the same purpose.

3.2.1

The Einstein Equation

Thermal diffusion and mass diffusion are both random processes that can be represented by random walks of particles. For the case of mass diffusion, the particles can be atoms, molecules or much larger entities such as colloidal particles or even unicellular animals. In the case of thermal diffusion, the particles are virtual heat “particles”. The century-old Einstein equation [2] describes the self-diffusivity D (or, equivalently, the thermal diffusivity K) of randomly walking particles in d dimensions ($d = 1, 2, 3$):

$$D = \frac{\langle R^2 \rangle}{2dt} \quad (3.1)$$

where R is the vector displacement of a *given* particle after some long time t and the Dirac brackets $\langle \rangle$ refer to an average over a very large number (N) of particles. It should be noted that the thermal conductivity λ_i in a phase i is directly related to the thermal diffusivity K_i in that phase by the well-known expression $K_i = \lambda_i / \rho_i C_p^i$, where ρ_i is the density of phase i and C_p^i is its specific heat. In a composite, by simply requiring that the densities and the specific heats take values equal to unity everywhere in the calculation, the effective thermal conductivity λ_{eff} then simply equals the effective thermal diffusivity K_{eff} . In the following, wherever the generic term “effective diffusivity” is used, the reader can freely substitute effective thermal conductivity or effective thermal diffusivity.

The Einstein equation refers only to a system already at equilibrium. In a mass diffusion context, the Einstein equation refers to the determination of the diffusivity of individual particles that can be followed or traced in a system that is already at chemical equilibrium, i.e. with no concentration gradient. In other words, *each* particle would need to be followed for some time t in order to determine its displacement R in that time. There are rather few examples where this has been possible to achieve in a real experiment. One example known to the authors makes use of a field ion microscope to follow or trace individual surface rhodium atoms diffusing on various faces of a face-centered cubic (fcc) rhodium crystal [3]. If the ad-atom fraction is low and the ad-atoms are observed frequently, then it is possible in effect to tag the atoms by noting at each observation which atom has moved, and how far, since the previous observation. The rhodium surface diffusivity itself can then be formed directly using Eq. (3.1) after a suitable diffusion time. To the authors’ knowledge, in a thermal diffusion context the Einstein equation has no physical meaning in the sense that it can be made use of experimentally. The Einstein equation purely provides a highly useful means for calculating in models the effective thermal diffusivity (conductivity) from random walks of virtual particles using the Monte Carlo method.

The Einstein equation has been extremely useful, especially for providing the basis for much of the theory that describes diffusion of atoms in the solid state, where it is commonly assumed that atoms jump from site to site on a lattice with

very long residence times on each site between jumps and an assumed flight time between sites of zero. (This is sometimes loosely referred to as the “hopping model”.) The atoms, individually and also their center of mass, undertake random walks on a lattice. In a period extending over half a century, a vast literature has been built up that has been especially concerned with describing memories or correlations between individual jumps of the random walk of primarily tracer atoms (see, for example, [4]). Since about the early 1970s, much of this literature has made use of the Monte Carlo method (see, for example, [5]). For random walks (say with correlations) on the simple cubic lattice the diffusivity can be partitioned from Eq. (3.1) as [4]

$$D = \frac{\Gamma f s^2}{6} \quad (3.2)$$

where Γ is the jump rate, s is the jump distance and f is termed the correlation factor, this quantity expressing any correlations in the directions of the jumps. If it is a square planar lattice then the factor 6 in the denominator of Eq. (3.2) is replaced by a factor 4. For a complete random walk, i.e. when each jump in the walk is completely independent or uncorrelated with all previous ones, then $f=1$. In contrast, for a hypothetical walk where every jump of the particles is immediately reversed, then $f=0$.

As an aside, it is worth noting that for many solid-state diffusion mechanisms, such as the vacancy mechanism, there are considerable correlations in the directions of successive jumps of the atoms because of the continued proximity of the vacancy to a tagged atom (tracer atom). For the vacancy diffusion mechanism the correlation factor is given approximately by

$$f \approx 1 - \frac{2}{Z} \quad (3.3)$$

where Z is the local coordination number.

It is very important to recognize that the Einstein equation (Eq. (3.1)) is still valid over long times even when the material has different hopping rates in different regions of the material (e.g. in a composite), *provided* that the material remains isotropic in its diffusion properties overall. If the material is anisotropic in its diffusion properties, one can still nonetheless define diffusivities in the three principal directions simply by using

$$D_x = \frac{\langle X^2 \rangle}{2t}; \quad D_y = \frac{\langle Y^2 \rangle}{2t}; \quad D_z = \frac{\langle Z^2 \rangle}{2t} \quad (3.4)$$

where X is the displacement of a particle in time t in the x -direction and so on.

The Einstein equation and the process of describing random walk diffusion of particles on a lattice lend themselves particularly well to Monte Carlo methods. Directing random walks of particles on lattices with random numbers was in fact

one of the first applications (1951) of the new Monte Carlo method that had been developed at Los Alamos during World War II as part of the Manhattan Project [6]. Perhaps surprisingly, the Einstein equation itself was not used until the early 1970s. A possible reason for this is the difficulty in dealing with time. In fact, in contrast to the other main kinetics simulation method of molecular dynamics, simulating actual time is not possible in a Monte Carlo kinetics calculation. What one actually does is to use a discrete quantity that is proportional to real time. This quantity is the number of jump attempts per particle. Using the Einstein equation with this quantity acting as “time”, one can then calculate a relative diffusivity, i.e. relative to one of the known diffusivities (usually the highest) in the system.

Let us see now how this might be achieved in a Monte Carlo calculation. First of all, we consider a very simple example where the diffusivity is the same everywhere. Consider then the case of diffusion of isolated particles on a simple cubic lattice having the dimensions, say, of $100 \times 100 \times 100$. There are six jump directions for each jump of a particle, i.e. the coordination is six. We suppose that this lattice has periodic boundaries. This very common type of boundary condition implies that when a particle reaches an edge or face of the lattice, if the next jump would take it outside of the lattice, then the particle is simply plugged back into the edge or face of the lattice directly on the opposite side of the lattice. In effect, with the imposition of periodic boundaries, the original lattice is now surrounded by periodic images or replicas of itself. The use of periodic boundaries thus enables surface effects to be avoided completely. However, the lattice is still a small system, and, if too small, historical effects may be perpetuated in some diffusion problems as a particle leaves one side and enters on the opposite side into what is, in effect, the same environment that it has just left. If problems such as diffusion in thin films are being addressed, a formal surface(s) is of course necessary and is retained in the calculation.

Monte Carlo methods require of course random numbers and a typical calculation requires many millions of them. Computer-generated random numbers r_i are generally calculated in most library subroutines in such a way that they are produced *uniformly* on the following interval: $0 \leq r_i < 1$. In our calculation here, a particle is created at some randomly chosen site (random numbers are used to generate the x , y and z coordinates for this site) and the direction to jump is also chosen at random (from the six available in this particular case where the simple cubic lattice is used). We could in fact release all N particles at exactly the same time at randomly chosen sites in the lattice and then start the simulation by choosing them randomly to jump. Provided that we permit multiple occupancy of a given site, the particles would diffuse independently of each other for the entire time Nt . As an alternative, we could release the particles one at a time, i.e. we let each one diffuse for exactly the same time t before the next one is released. Both of these procedures are completely equivalent at long times and would take about the same amount of computational time, but the second way is slightly easier conceptually and we will assume it in the following.

Whilst the random walk of the particle is being directed by the computer-generated random numbers, step-by-step contributions to the vector displacement

of the particle R are also being accumulated. It has been found that it is probably best to do this by assuming that each particle starts from its own origin $(0, 0, 0)$. It should be especially noted that if the particle crosses a periodic boundary and is therefore plugged into the opposite side of the lattice, this process is completely ignored in the calculation of R . The process of directing the random walk of the particle continues for, say, 5000 jump attempts. The entire process is then repeated with further particles until, say, a total of $N = 10^6$ particles have been released, all having had 5000 jump attempts in their walks. In this particular example, every attempt to jump is permitted to be successful (this is equivalent to saying that the jump frequency $\Gamma = 1$ jump per jump attempt of the particle). The jump distance here $s = 1$ lattice spacings. Since $f = 1$ here (the particles diffuse completely independently), Eq. (3.2) shows immediately that D should equal $1/6$ and also carries the units of lattice spacings squared per jump attempt. A calculation of D directly from the Monte Carlo calculation using the Einstein equation (Eq. (3.1)) verifies this perfectly. The value here of $1/6$ taken by D then must be scaled to the actual diffusivity in the material.

Now let us consider diffusion in a simple two-component composite material. For the sake of concreteness, we consider the dispersed phase (the inclusions) to be spheres (region 2) that are embedded in a matrix phase (region 1) and that the spheres are themselves arranged for convenience here in a simple cubic arrangement. We assume that the diffusivity in the spherical inclusions themselves is D_2 and that the diffusivity in the matrix is D_1 . We are then interested in calculating the effective diffusivity D_{eff} of the composite. As a very rough approximation for the effective diffusivity in a composite, we can write the effective diffusivity as a simple linear combination of the individual diffusivities:

$$D_{\text{eff}} = gD_2 + (1 - g)D_1 \quad (3.5)$$

where g is the volume fraction of the inclusion phase. In the solid-state diffusion literature, Eq. (3.5) is commonly referred to as the Hart equation [7] and refers to the specific situation in that area of materials science where the two components are the bulk (the grains) and the grain boundary “phase”. Equation (3.5) is exact only when the two phases or regions are parallel and the diffusivities are measured in that direction.

A Monte Carlo determination of the actual effective diffusivity in a composite consisting of spherical inclusions in a simple cubic arrangement can be simply achieved in the following way. A fine-grained simple cubic lattice say $(100 \times 100 \times 100)$ is overlaid on this system as shown schematically in two-dimensional (2D) form in Figure 3.1. This lattice needs of course to be sufficiently fine grained that it can adequately capture the shape of the spherical inclusions. The volume fraction of inclusions is simply the number of lattice sites in the inclusion(s) divided by the total number of sites. The lattice also has periodic boundaries which are implemented exactly as in the simple system described above. Since the system has periodic boundaries, it does not actually matter in this particular example if the inclusion is in the center of the lattice because the arrangement of the spherical inclusions is also simple cubic. Recall that with the employment of periodic boundaries, the

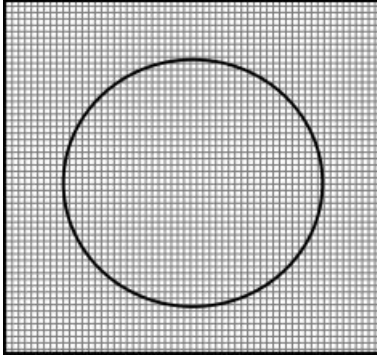


Figure 3.1 A 2D model of a composite of spherical inclusions in a simple cubic arrangement overlaid by a simple cubic lattice that is then explored randomly by a large number of virtual particles.

lattice is surrounded by images of itself. For more complicated arrangements of the inclusions in the lattice, which essentially acts like a unit cell of the structure of the chosen arrangement, the inclusions must be located with care.

As in the earlier example described above, a single particle is created and released from a randomly chosen site in the lattice. There are absolutely no correlation effects here to be concerned with because the particle is diffusing completely independently of others. The two diffusivities D_1 and D_2 are now simply individually represented by the two (different) jump rates Γ_1 and Γ_2 . It is usual to scale the higher jump rate to unity for computational efficiency. The jump rate of the particle now varies according to position within the lattice. Thus if the particle is currently on a site known to be in region 1 (i.e. the spherical inclusion), it has a jump rate Γ_1 , whereas if the particle is currently on a site known to be in region 2, then it has a jump rate of Γ_2 . As an example, let $\Gamma_1 = 1$ and $\Gamma_2 = 0.1$ (this means that the ratio of the diffusivities $D_1/D_2 = 10$). Thus when the particle is on a “region 2 site”, another random number r needs to be generated to determine the outcome of the jump attempt. If r is greater than Γ_2 then this jump attempt is said to have failed and a *jump direction* must again be chosen at random for this particular particle. (Note that if the simulation is being done in such a way that all particles were released at the same time, then if an attempt to jump is unsuccessful, a particle must again be chosen at random from the cohort.) If r is less than or equal to Γ_2 then the jump attempt is said to have been successful and the particle is permitted to change sites. As in the simple example above, after a large number of particles have been released, say $N = 10^6$, then the effective diffusivity for the composite can be formed directly from Eq. (3.1). The effective diffusivity of the composite is automatically scaled relative to the highest diffusivity (in this particular case, to that of the matrix D_1). It is clear that it is very easy to introduce other inclusions having different diffusivities into the matrix. It is also straightforward to allow position-dependent diffusivities even within the inclusions or the matrix by simply mapping such dependencies onto the corresponding jump frequencies Γ_i . This method of calculating the effective diffusivity is basically a

finite difference method for the solution of the corresponding inverse diffusion equation (see, for example, Manning's [8] derivation of the Einstein relation Eq. (3.1) with the diffusion equation as a starting point).

The principal difficulty in the Monte Carlo calculation of the effective diffusivity is ensuring that the number of jump attempts is sufficiently large to ensure that the long-time effective diffusivity of the composite is in fact correctly determined. At very short diffusion times for each particle, as might be expected, the effective diffusivity is simply given by the approximate Eq. (3.5) because this would be the *instantaneous* effective diffusivity. At very long diffusion times, after each particle has adequately "explored" the structure, the correct long-time limit effective diffusivity of the composite is obtained (see Fig. 3.2). As a good guide to what would be a sufficiently long time, it is best to first form the effective diffusivity according to the approximate Eq. (3.5) and then use this via the "diffusion length", $(6D_{\text{eff}}t)^{1/2}$, to determine the number of jump attempts (t) appropriate for the problem. As a reasonable guide, the diffusion length should be at least half the length of the lattice, or unit cell of the ordered structure of the inclusions.

In some applications, one may wish to introduce some degree of randomness to the arrangement of the inclusions or to their size, or possibly their shape. This poses no major problems. For the purposes of changing the arrangement of the inclusions, at one extreme, one may start from an ordered arrangement of the inclusions which is then randomized to some extent by making appropriate random shifts of the inclusions within the lattice but without allowing the inclusions to overlap. At the other extreme, one might first prepare a gas-phase like distribution or even a dense random packing distribution [9] of the inclusions in a separate calculation. This distribution is then mapped onto a fine-grained lattice. In both cases, the effective diffusivity is still determined simply as described above from the Einstein

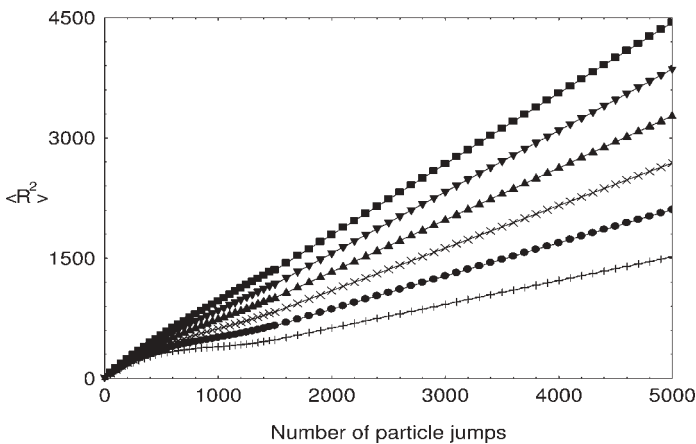


Figure 3.2 Convergence of the mean square displacement versus number of jumps of virtual particles – simple cubic ordered arrangement of spheres at various porosities ε : ■ = 0.82; ▼ = 0.62; ▲ = 0.48; × = 0.33; ● = 0.20; + = 0.10 [9].

equation [9]. Of course in most cases it will also be necessary to average over a number of starting random distributions of the inclusions in order to obtain a reliable estimate of the effective diffusivity of the composite model being dealt with. Dealing with a distribution of sizes of the inclusions is straightforward and needs no explanation. Inclusions taking the standard geometrical shapes of spheres, cubes, ellipses, etc., are, of course, straightforward to implement. In principle, actual experimental inclusion shapes could be mapped onto the lattice making use of image analysis of micrographs from a confocal microscope and then the effective diffusivity determined.

As noted above, the highest jump frequency (diffusivity) is scaled to unity for efficiency. When one of the diffusivities is very small, the Monte Carlo method with the basic algorithm described above frequently tends to run into difficulties arising from rather large computational inefficiency (most attempts to jump are rejected in that region) and a slight nonrandomness in the random number generation and the subsequent inhomogeneity of the random numbers generated over the range zero to unity. This will be magnified for diffusion in the slow diffusivity region. These difficulties can be avoided or at least minimized by making use of straightforward residence time algorithms as documented in related Monte Carlo lattice calculations (see, for example, [10]). Such algorithms can be very useful when the diffusivities vary by many orders of magnitude. A popular choice makes use of an algorithm that guarantees a jump on every attempt [11] wherein the particle's site residence time (the reciprocal of the jump frequency) is simply added to the elapsed time at each move. In principle, this can lead to overshooting of the specified time, although this is unlikely to be a serious problem at very long diffusion times. There is, of course, a significant computational overhead with such algorithms that may offset some of the efficiency gains.

3.2.2

Fick's First Law (Fourier Equation)

As an alternative to the Einstein equation for the calculation of the effective diffusivity, it is also possible to make use of Fick's first law in a steady-state condition [12]:

$$J = -D \frac{\partial C}{\partial x} \quad (3.6)$$

In this problem, Fick's first law for the mass particle flux is equivalent to Fourier's law for the heat particle flux. In Eq. (3.6), J is the particle flux and $\partial C/\partial x$ is its concentration gradient. Equation (3.6) is most conveniently used under steady-state conditions by introducing a source plane, on which particles can be created at a random position and released one at a time, and a sink plane, at which the particles are annihilated as soon as they arrive. This of course gives an apparent particle concentration of $1/n$ for the source plane (where n is the number of sites on that plane) and zero for the sink plane. This, along with the length of the lattice between

the source plane and the sink plane, provides the uniform concentration gradient $\partial C/\partial x$. This gradient can also be adjusted by changing the length of the lattice or by adjusting the probability for the particle being annihilated at the sink plane. For example, if a particle arrives at the sink plane and is annihilated with a probability of P_i (appropriately evaluated on the spot using a new random number), the effective concentration of particles on that plane is then simply given by $(1 - P_i)/n$ and the concentration gradient in the problem is thus reduced. The source and sink planes are separated by some 100 planes in the $+x$ direction and by the same number of planes via the periodic boundary in the $-x$ direction. A particle is released from the source plane and is permitted to diffuse to the sink, thereby providing, in effect, a well-defined uniform concentration gradient. The flux J is simply calculated as the *net* number of particles that have crossed between two neighboring planes in the x -direction as calculated over a long time t during which some 10^5 particles are released from the source and annihilated at the sink. Inclusions are introduced in exactly the same way as the Einstein equation method described above and diffusion is simulated in the same way. However, it should be noted that a particle may see in effect only one isolated inclusion in its lifetime in going from source to sink and give an incorrect result for the effective diffusivity. For this reason, periodic arrangements of inclusions would require at least two inclusions between the source plane and the sink plane of particles.

Results of calculations of the effective thermal conductivity in simple 2D composites via the Einstein equation and Fick's first law have been shown to be in very good agreement [12]. In general, however, it must be said that for calculating the effective diffusivity, the Einstein equation method is considerably easier to use than the Fick's first law method and, furthermore, is much more flexible in its application. The authors doubt if the Fick's first law method in general has any particular advantages over the Einstein equation method and therefore probably remains largely of pedagogical interest.

3.3

Monte Carlo Calculations of the Effective Thermal Conductivity

In this section, we summarize most of the published Monte Carlo results on the effective diffusivity in models of composites and porous media. Many of the results have been published in the form of effective mass diffusivities. As shown in the previous section, these are simply equivalent to effective thermal diffusivities, and, if we let the densities and specific heats be equal everywhere, these are also equivalent to the effective thermal conductivities too.

3.3.1

Effective Diffusion in Two-Component Composites/Porous Media

The first Monte Carlo calculation of the effective diffusivity was concerned with determining the effective diffusivity of the void space of a simple model of porous

media that was constructed from spheres [9]. Although a large analytical theory literature exists on this subject (see, for example, the reviews by German [13] and Torquato [14] and several contributions to the present volume), the various derived expressions had never been tested against well-defined models and exact (numerical) calculations. Various ordered (fcc, body-centered cubic (bcc) and simple cubic (sc)) and random packing arrangements of impermeable spheres were examined in that first Monte Carlo study. Random distributions of touching spherical particles were generated in the following way. First, spheres were introduced randomly into a volume (nonperiodic) without overlap. In order to generate dense random packing of the spheres there are quite a number of possible algorithms available (see, for example, Torquato [14]). However, it is generally accepted that the dense random packing of spheres always depends slightly on the actual algorithm used and that there may in fact be no perfect algorithm for generating dense random packing [14]. In the Monte Carlo study [9], dense random packing of spheres was obtained by starting with a very simple Lennard-Jones pair-potential between particles that was tailored to have a very dominant repulsive part of the potential; this was intended to closely approximate hard spheres and a very weak attractive part of the potential. The potential energy function for the system of spheres was then minimized by taking very small fixed spatial steps of the spheres in random directions. This minimization procedure tends to avoid collapsing to the most stable fcc arrangements which is a frequent difficulty when standard numerical minimization techniques are employed with spheres of equal size. Arrangements of “spheres” at densities higher than dense random packing were generated in the study by the simple artifice of simply enlarging the spheres further after minimization, thereby in effect overlapping the spheres. In addition, the case of equal concentrations of spheres of two different sizes was also examined in dense random packing arrangements.

Once the densely randomly packed arrangement of spheres had been prepared it was overlaid with a fine-grained grid with a mesh size of typically 100 spacings per sphere diameter as described in general terms in Section 3.2.1. The effective diffusivity of the void space ε (equal to $(1 - g)$) between the spheres was obtained according to the Einstein equation as described in Section 3.2.1. The diffusivity within the spheres was assumed to be zero. Typical behavior of the convergence of the effective diffusivity with time (shown here as particle jumps) for different porosities is shown in Figure 3.2, in this case for a random distribution of mono-sized spheres. In the study, the results for both ordered and random arrangements of spheres were compared with a number of analytical expressions for the effective diffusivity. In both ordered and random cases, it was found that the effect of arrangement of the spheres on the diffusivity of their corresponding void space is fairly slight, i.e. the arrangement of the spheres appears to have only a second-order effect on the value taken by the effective diffusivity.

The analytical expression for the effective diffusivity due to Maxwell [15,16], which was later derived in a rather more general way by Neale and Nader [17],

$$\frac{D_{\text{eff}}}{D_1} = \frac{2\varepsilon}{3 - \varepsilon} \quad (3.7)$$

appears to act as an upper bound for the effective diffusivity whilst the analytical expression derived by Bruggeman [18],

$$\frac{D_{\text{eff}}}{D_1} = \varepsilon^{3/2} \quad (3.8)$$

appears to act as a lower bound for the effective diffusivity, but there is little overall pattern emerging between these limits probably because of an unfortunate small statistical uncertainty in this early Monte Carlo calculation. A third expression for the effective diffusivity, derived by Prager [19] is

$$\frac{D_{\text{eff}}}{D_1} = \varepsilon \left(1 - \frac{1 - \varepsilon}{2} \right) \quad (3.9)$$

which gives a behavior for the effective diffusivity that is roughly halfway between the other two. Figure 3.3 shows the behavior of the effective diffusivity as a function of porosity for the case of random distributions of spheres of two different sizes.

We mention here another pioneering Monte Carlo study of the effective mass diffusivity in 2D models of a composite composed of circular and square inclusions for the condition where the concentration of diffusant in the inclusions was equal to zero [20]. As a result of this condition, the results in this case do not map readily across to the thermal diffusivity.

The next Monte Carlo study [21,22] was put into the context of the effective mass diffusivity in nanomaterials where diffusion occurs via both the grains (nanocrystals)

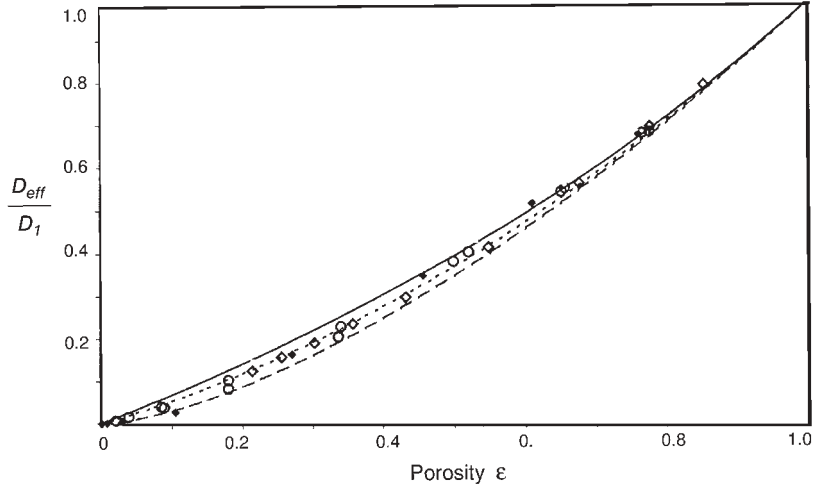


Figure 3.3 The ratio D_{eff}/D_1 as a function of porosity ε for various random arrangements: $\circ$ = mono-sized spheres; $\blacklozenge$ = equal numbers of spheres (one of which is 0.8 times the diameter of the other); $\diamond$ = equal numbers of spheres (one of which is 0.4 times the diameter of the other). Solid line corresponds to Eq. (3.7); dashed line corresponds to Eq. (3.8); dotted line corresponds to Eq. (3.9) [9].

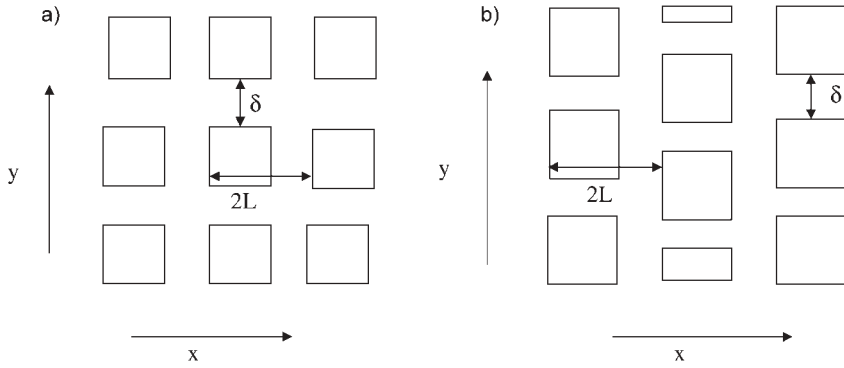


Figure 3.4 Schematic representation of two-dimensional composite model comprising: (a) low diffusivity square grains in a square planar arrangement surrounded by a high diffusivity (grain boundary) interfacial region; (b) low diffusivity square grains in a brickwork-type arrangement surrounded by a high diffusivity (grain boundary) interfacial region.

and the interface regions (grain boundaries). Two very simple 2D square grain configurations were examined which are shown in 2D form in Figures 3.4a and b. The particular situation that is relevant to this context is where the grain boundary diffusivity is considerably larger than the diffusivity within the grains. Putting this into the parlance of a two-component composite this situation would be equivalent to one where the diffusivity of the matrix phase is considerably larger than the diffusivity of the (square) inclusions. The model was overlaid by a fine-grained grid in the usual way as described in Section 3.2.1. The effective diffusivity was calculated according to the Einstein equation. The results were compared to several derived expressions. Easily the best expression of these (for both models) was derived by treating the diffusion problem as one having two parallel effective diffusion paths: one path simply corresponds to those grain boundaries parallel to the diffusion direction whilst the other path consists of those grain boundaries normal to the diffusion direction and the grains themselves. Analysis of this situation gives the following equation:

$$\frac{D_{\text{eff}}}{D_1} = \frac{(\sqrt{1-\varepsilon} - 1 + \varepsilon)D_1 + (2 - \sqrt{1-\varepsilon} - \varepsilon)D_2}{\sqrt{1-\varepsilon}D_1 + (1 - \sqrt{1-\varepsilon})D_2} \quad (3.10)$$

An extension that differentiates between the two directions for the brickwork case $g \leq 0.75$ (Figure 3.4b) gave the following expressions for the effective diffusivities in the y- and x-directions:

$$\begin{aligned} \frac{D_{\text{eff}}^y}{D_1} &= \frac{(\sqrt{1-\varepsilon} - 1 + \varepsilon)D_1 + (2 - \sqrt{1-\varepsilon} - \varepsilon)D_2}{\sqrt{1-\varepsilon}D_1 + (1 - \sqrt{1-\varepsilon})D_2} \\ \frac{D_{\text{eff}}^x}{D_1} &= \frac{(\sqrt{1-\varepsilon} - 1 + \varepsilon)D_1^{\text{eff}} + (2 - \sqrt{1-\varepsilon} - \varepsilon)D_2}{\sqrt{1-\varepsilon}D_1^{\text{eff}} + (1 - \sqrt{1-\varepsilon})D_2} \end{aligned} \quad (3.11)$$

where

$$D_1^{\text{eff}} = \frac{4D_1}{9 - 4\varepsilon - 4\sqrt{1 - \varepsilon}}$$

These relations provide a significant improvement in this range of the fraction of inclusions. Figure 3.5 shows a comparison of the Monte Carlo data with Eq. (3.10) for

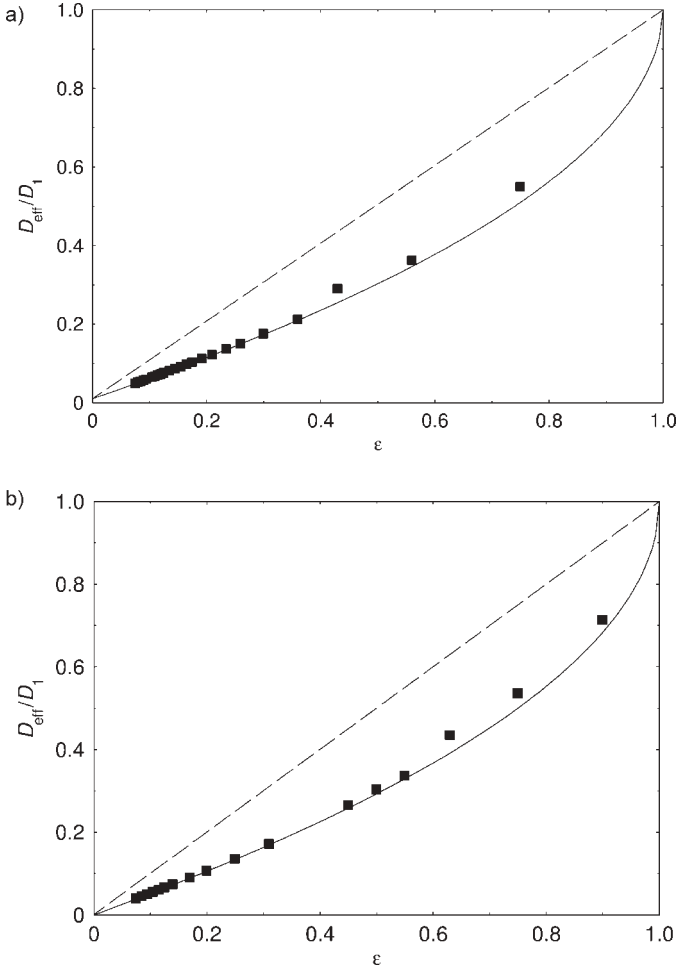


Figure 3.5 Ratio of the effective diffusivity to the matrix diffusivity as a function of porosity ε ($= 1 - g$), g is the volume fraction of the dispersed phase for the case of squares in a square planar arrangement. Data points are Monte Carlo results, solid lines represent the estimate (Eq. (3.10)), dashed lines represent estimate by Eq. (3.5). Ratio of the grain boundary diffusion to the bulk (lattice) diffusion is (a) 10^2 , (b) 10^3 and (c) 10^4 .

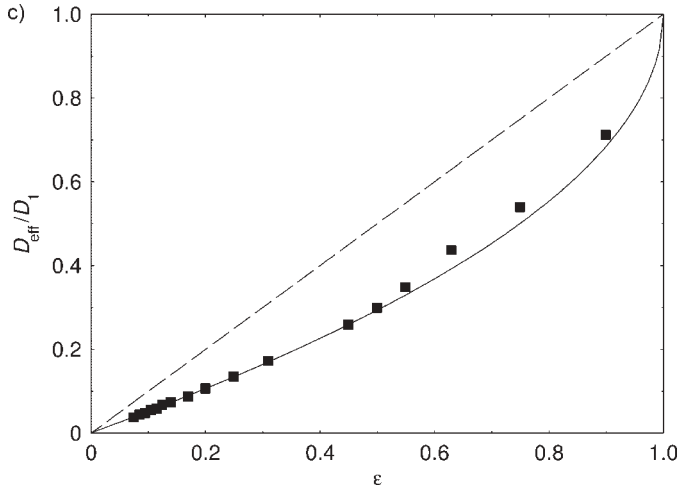


Figure 3.5 (legend see p. 85).

the effective diffusivity for the model of Figure 3.4a (square planar arrangement of square inclusions). It can be seen that Eq. (3.10) does very well indeed compared with the weighted average of the diffusivities, the Hart equation (Eq. (3.5)). Note that this arrangement of inclusions does not have a percolation threshold.

A Monte Carlo study closely related to the above examined the effective diffusivity for a model of cubic grains in a simple cubic arrangement [23]. Again the relevant case where the diffusivity in the grain boundaries is much greater than that in the grains was examined. Over the entire grain boundary fraction range it was shown that the appropriate equation for the thermal diffusion version of the Maxwell-Garnett equation

$$\frac{D_{\text{eff}}}{D_1} = \frac{2(1-g)D_1 + (1+2g)D_2}{(2+g)D_1 + (1-g)D_2} \quad (3.12)$$

does very well indeed in describing the effective diffusivity for this model. The equation derived especially for this three-dimensional (3D) geometry (similar to Eq. (3.10)) does almost as well too. It was found that Eq. (3.12) gives better agreement with the Monte Carlo simulation results when grain boundaries are relatively thick and allowed more than 10 atomic jumps across (in effect represented by the lattice here). In contrast, if grain boundaries are thin and only up to 5 atomic layers across then the Monte Carlo simulation results agree better with the 3D analogue of Eq. (3.10).

A later and quite comprehensive Monte Carlo study of the effective diffusivity in two-component composites examined the effective diffusivity for a simple model of dispersed *spherical* inclusions in fcc, bcc and sc arrangements [24]. In that study, two cases of the relative diffusivities were examined: (1) the diffusivity of the inclusions

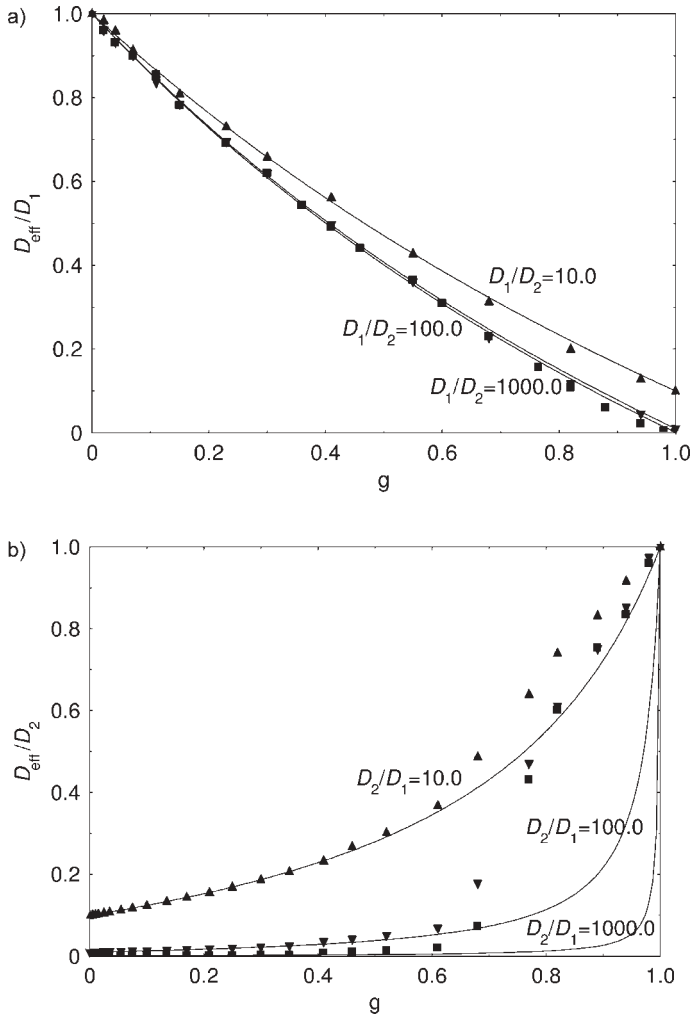


Figure 3.6 (a) D_{eff}/D_1 as a function of the volume fraction g of the second phase for the case of a bcc type of arrangement of spheres for three ratios of D_1/D_2 : $\blacktriangle = D_1/D_2 = 10$; $\blacktriangledown = D_1/D_2 = 10^2$; $\blacksquare = D_1/D_2 = 10^3$. Solid lines correspond to Eq. (3.12). (b) D_{eff}/D_2 as a

function of the volume fraction of the second phase for the case of a bcc type of arrangement of spheres for three ratios of D_2/D_1 : $\blacktriangle = D_2/D_1 = 10$; $\blacktriangledown = D_2/D_1 = 10^2$; $\blacksquare = D_2/D_1 = 10^3$. Solid lines correspond to Eq. (3.12).

is less than the matrix phase, and (2) the diffusivity of the inclusions is greater than the diffusivity of the matrix phase. Results for the effective diffusivity for bcc and fcc arrangements are shown in Figure 3.6a and b and Figure 3.7a and b, respectively. Note that the entire density range, i.e. above the percolation threshold $g = 0.68$ and 0.74 (where the spheres touch for fcc and bcc arrangements, respectively), is covered in that study by simply allowing the diameters of the spheres to increase and so for

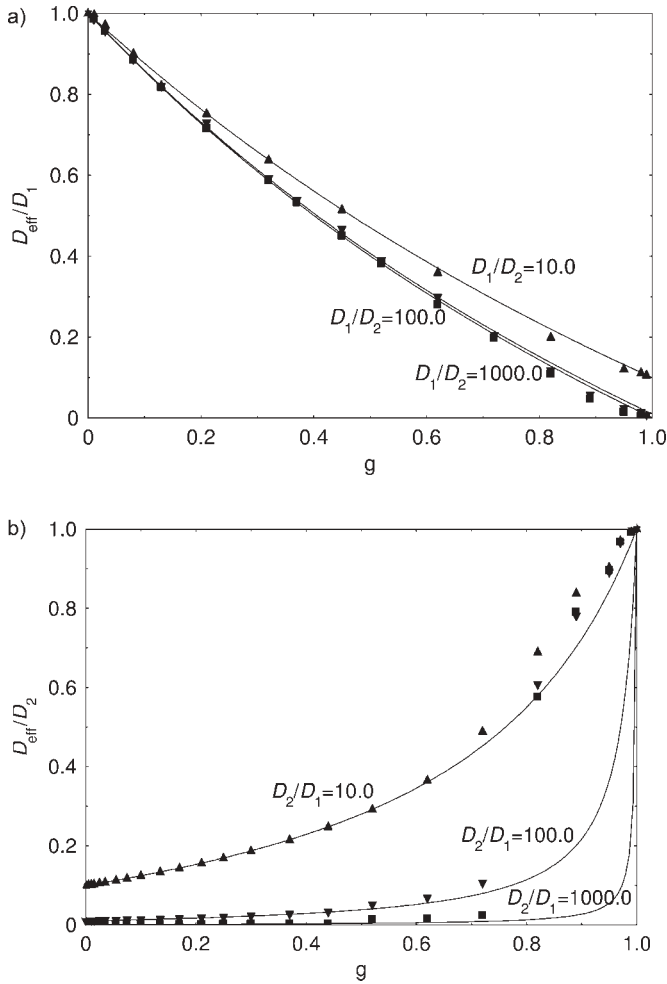


Figure 3.7 (a) D_{eff}/D_1 as a function of the volume fraction of the second phase for the case of a fcc type of arrangement of spheres for three ratios of D_1/D_2 : $\blacktriangle = D_1/D_2 = 10$; $\blacktriangledown = D_1/D_2 = 10^2$; $\blacksquare = D_1/D_2 = 10^3$. Solid lines correspond to Eq. (3.12). (b) D_{eff}/D_2

as a function of the volume fraction of the second phase for the case of a fcc type of arrangement of spheres for three ratios of D_2/D_1 : $\blacktriangle = D_2/D_1 = 10$; $\blacktriangledown = D_2/D_1 = 10^2$; $\blacksquare = D_2/D_1 = 10^3$. Solid lines correspond to Eq. (3.12).

the spheres to overlap extensively. It was found that for the values of the individual diffusivities the Maxwell-Garnett equation, Eq. (3.12), does very well in describing the effective diffusivity up to the percolation threshold where the spheres touch. Above this threshold, the Monte Carlo results increasingly deviate from the predictions of the Maxwell-Garnett equation. This deviation is of course not unexpected since the derivation of the Maxwell-Garnett equation explicitly makes the assumption that

the inclusions are *not* continuous [15,16]. It can also be seen by comparing Figures 3.6 and 3.7 that the arrangement of the spheres does not have a strong effect on the values taken by the effective diffusivity.

The problem of determining and analyzing the effective diffusivity in a material that has contributions from grain and grain boundary diffusion was reviewed [25] and some further Monte Carlo data were included in that review. Special emphasis was put on the limits of usefulness of the Hart and Maxwell-Garnett equations. Comparison of the Monte Carlo data of the effective diffusivity of cubic and spherical grain models (the diffusivity was always assumed to be greater in the grain boundaries) showed that the Maxwell-Garnett equation consistently provides a superior description of the effective diffusivity than the Hart equation unless the diffusion time is sufficiently small that the problem can be conceived as diffusion only along parallel paths extending in from the surface. Again it was noted that for the special case of cubic grains in a simple cubic arrangement with thin grain boundaries from 2 to 5 atomic layers across the 3D version of Eq. (3.10), which better takes into account the actual geometry of the grains, provides better agreement with the Monte Carlo data than the Maxwell-Garnett equation.

A very detailed comparison of Monte Carlo and finite element calculations of the effective diffusivity (expressed in that paper as the effective conductivity) of circular and square inclusions both in square planar arrangements was undertaken by Fiedler *et al.* [12] for the case where the diffusivities of the matrix and inclusions differ by up to an order of magnitude. Both cases of the inclusions having a higher and lower diffusivity than the matrix were examined. Excellent agreement for the effective diffusivity is found between these quite different methods. Results for the effective diffusivity are shown in Figure 3.5a and b for the cases of circular and square inclusions, respectively. It was also shown in that study that the results are in excellent agreement with the Maxwell-Garnett equation, Eq. (3.12), except in the case of the circular inclusion fractions above the percolation threshold (i.e. where the circular inclusions already touch).

Finally in this section, we mention a detailed study of the effective diffusivity for the case of 2D square inclusions arranged in square planar and brickwork patterns where the inclusions have a diffusivity three orders of magnitude less than that of the matrix phase [26]. It was shown that the Maxwell-Garnett equation describes this extreme situation roughly but for an accurate representation of the effective diffusivity it is necessary to take into account the actual arrangement of the dispersed phase. This means that Eq. (3.11) should be used for the brickwork pattern and Eq. (10) for the square planar arrangement.

In summary, one can say that for these very simple models of two-component composites the basic Maxwell-Garnett equation always provides quite a reasonable description of the effective diffusivity. It probably best describes the effective diffusivity when the diffusivities of the components are relatively close, say within about an order of magnitude. In such a situation the actual arrangement of the inclusions is not very important. But for more extreme ratios of the diffusivities it is better to use equations such as Eqs. (3.10) and (3.11) which take explicit account of the actual geometrical arrangement of the inclusions. Analytical expressions that are

analogous to Eqs. (3.10) and (3.11) can be readily derived for other shapes of the inclusions.

3.3.2

Effective Diffusion in Three-Component Composites

The problem of determining the effective diffusivity in three-component composites has also been addressed with Monte Carlo methods again making use of a fine-grained lattice that is overlaid onto the problem. The first Monte Carlo calculation [27] was couched in terms of determining the effective diffusivity in a material containing two alternating (in all directions) stable cubic phases (A and B with diffusivities D_A and D_B and volume fractions g_A and g_B , respectively) that are separated by interphase boundaries (C) of high diffusivity D_C . A general expression for the thermal conductivity in a model of a three-phase material was derived many years ago by Brailsford and Major [28]. The same expression was derived in a more general way [26] to include possible segregation of the diffusant in the various phases. The original expression of Brailsford and Major [28] is

$$\frac{D_{\text{eff}}}{D_C} = \frac{1 - 2g_A \frac{D_C - D_A}{2D_C + D_A} - 2g_B \frac{D_C - D_B}{2D_C + D_B}}{1 + g_A \frac{D_C - D_A}{2D_C + D_A} + g_B \frac{D_C - D_B}{2D_C + D_B}} \quad (3.13)$$

Two other equations for the effective diffusivity were also derived [27] using Maxwell-type arguments in succession. The Monte Carlo results for the effective diffusivity show that the effective diffusivity in the composite is certainly described roughly by Eq. (3.13). However, the detailed pattern of behavior of the effective diffusivity is rather complicated in this model: the other expressions give better agreement but in different ranges of the individual diffusivities and fractions of inclusions. At the present time, it is not possible to guide, at least in general terms, the choice for the best overall expression for the effective diffusivity.

Electrical (ionic) conductivity in three-phase composites in which an insulating phase (region 2) is embedded in an ionically conducting matrix (region 1) has recently been of great interest for enhancing the overall electrical ionic conductivity of the material. Such materials are frequently called “composite electrolytes”. Because of space charge effects immediately around the insulating phase, a “phase” (region 3) having a much higher electrical conductivity is present immediately around the insulating phase. There are two percolation thresholds: one where the highly conducting regions overlap and, later at high inclusion fractions, a second one where the insulating regions start to overlap. The problem is then to determine the effective ionic conductivity of this three-“phase” composite. This has been modeled by Monte Carlo methods using a similar procedure to that described above [29]. An approximate expression for the effective diffusivity was derived using Maxwell-type arguments. This was in better agreement with the Monte Carlo method than expressions derived in previous treatments.

3.4

Determination of Temperature Profiles

In this section, we demonstrate the use of the Monte Carlo method for determining temperature profiles in thermal transport problems involving composites. To our knowledge, no results for this situation have been published so far but concentration profiles in materials where the mass diffusivity depends on position have been published on quite a few occasions (see, for example, [25]). Obtaining the temperature (or concentration profile) is equivalent to solving the heat equation or diffusion equation by Monte Carlo methods for the designated initial and boundary conditions. In order to demonstrate the procedure we will focus first on two simple cases where the diffusivity is the same everywhere in the material. (Both cases have very well-known analytical solutions for the case when the solid is semi-infinite and the diffusivity does not depend on position.) Case 1 refers to a situation where there is a short pulse of heat “deposited” at the surface at time $t = 0$ which is then permitted to diffuse out into the material for some diffusion time t . This is formally equivalent to the well-known thin-film condition or instantaneous source for the diffusant that is commonly used in tracer diffusion experiments in the solid state. Case 2 refers to a situation where the temperature is held constant at the surface for the entire diffusion time t . This is formally equivalent to a diffusant in the gas phase (which is assumed to be an inexhaustible source of the diffusant) which then diffuses into the material for a given diffusion time.

The basic Monte Carlo procedure has a great many similarities to that described in Section 3.2. We first illustrate the procedure with case 1. A source plane of particles is established in the center of a large periodic simple cubic lattice in order to avoid edge effects in the calculation. Particles are generated at random positions on this source plane and released from the plane either sequentially or all at once. Assuming the latter for convenience here, we allow the particles to diffuse independently of one another for the entire time Nt , at which time the final position of each particle is recorded. The final positions of all of the particles, say 10^6 , are then simply assembled from the individual final positions to form a penetration profile. For mass diffusion, this is a concentration profile; for thermal diffusion, it is a temperature profile. If the lattice is large in the diffusion direction, at relatively short times, the profile is a simple Gaussian profile as appropriate for diffusion into an “infinite” solid. Several typical profiles obtained in this way are illustrated in Figure 3.8.

Case 2 requires a constant source of particles at the “surface” for all diffusion times and is obtained in the following way. The basic idea is simply to keep the total number of particles at the source plane constant at, say, 10^5 at all diffusion times. This is achieved in the following way. All particles are released at the same time. As each particle makes a jump from the source plane it is immediately replaced by a new one, which is again generated at a random position on this plane in order to maintain the number designated (10^5). Whenever a particle returns to the source plane, thereby exceeding the number designated (10^5) for the source, then that particle is permanently removed from the system. Over a period of time, the number of particles within the system naturally increases as more particles diffuse away from

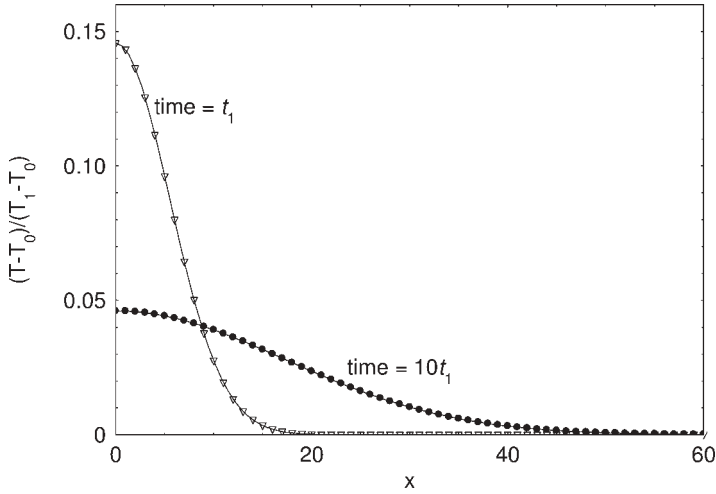


Figure 3.8 Typical Gaussian profiles for thermal diffusion from an instantaneous source for two different times (symbols represent Monte Carlo simulation results).

the source than return to it. Accordingly, the diffusion time t must be constantly re-scaled since the time is required to be proportional to the number of attempts per particle. An example of several profiles obtained in this way is shown in Figure 3.9. At longer times, the two profiles from each side of the source start of course to meet

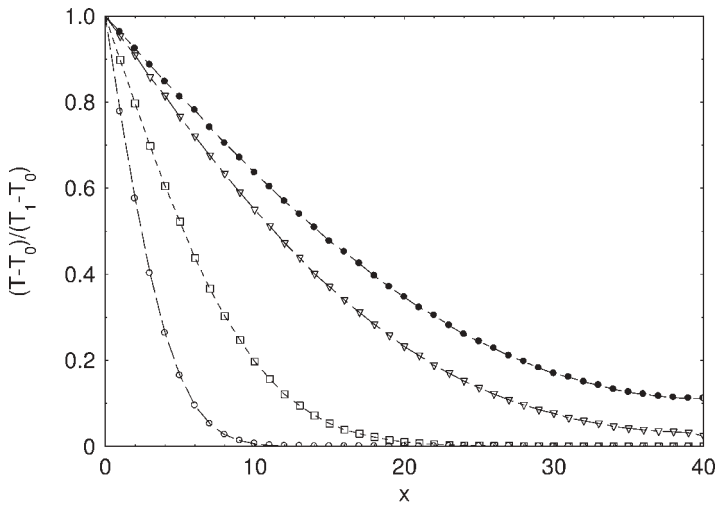


Figure 3.9 Temperature profiles from the two constant-temperature T_1 sources at $x=0$ and $x=80$ cm. T_0 is an initial temperature inside the single-phase material. Thermal diffusivity is $0.25 \text{ cm}^2 \text{ s}^{-1}$. Symbols represent Monte Carlo simulation results for different times: $\blacktriangledown = 25.5 \text{ s}$; $\square = 120.4 \text{ s}$; $\bullet = 560.7 \text{ s}$; $\triangledown = 890.5 \text{ s}$.

up via the periodic boundary. However, if the particle source is then conceived as two “separated” surfaces, then the profile represents diffusion from two surfaces into a material of a finite width.

In order to obtain temperature profiles in a composite it is quite a simple matter to include inclusions having a different jump rate from the matrix as described in detail in Section 3.2.1. Then the temperature profile or, indeed, a temperature

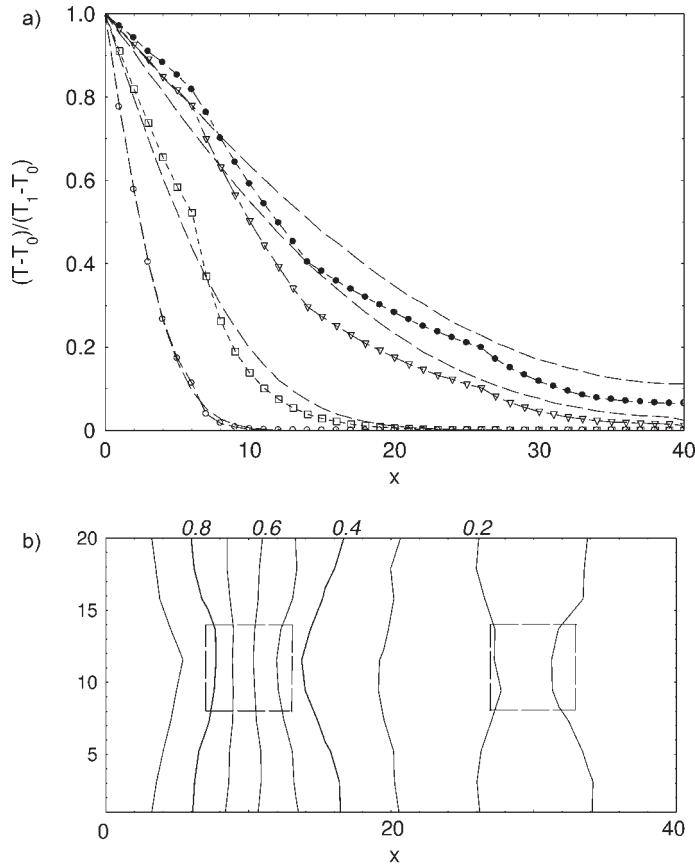


Figure 3.10 (a) Average temperature profiles from the two constant-temperature T_1 sources at $x=0$ and $x=80$ cm. T_0 is an initial temperature inside the two-phase material. Square inclusions in a square planar arrangement located between $x=6$ and $x=15$ and between $x=26$ and $x=35$. Thermal diffusivity of the inclusions is an order of magnitude lower than that of the matrix (thermal diffusivity of the matrix is $0.25 \text{ cm}^2 \text{ s}^{-1}$). Dashed lines represent the corresponding complementary error

function solution. Symbols represent Monte Carlo simulation results for different times: $\blacktriangledown = 25.5 \text{ s}$; $\square = 121.4 \text{ s}$; $\bullet = 593.3 \text{ s}$; $\nabla = 957.4 \text{ s}$. (b) Isothermal contour map for the two-phase media. Thermal conductivity of the inclusions is an order of magnitude lower than that of the matrix. The square inclusions are outlined with dashed lines. The time equals 957.4 s . The numbers in italics show the corresponding values of $(T - T_0)/(T_1 - T_0)$ isotherms.

contour map can be readily established. Examples of such profiles are shown in Figure 3.10a along with a contour map (Figure 3.10b) corresponding to the long diffusion time for a 2D case where the diffusivity in the square inclusions is less than that of the matrix.

In principle, it is possible to determine the effective diffusivity (conductivity) of a model composite by analyzing the temperature profiles. This would assume that there has been averaging of the profile over all possible locations of the inclusions. The profile would then be processed to give the effective diffusivity in much the same way as an experimental temperature profile or diffusant concentration profile by using the appropriate solution to the heat equation or diffusion equation, respectively. In practice, it is much easier to calculate the effective diffusivity of the model composite in a separate calculation using the Einstein equation along the lines of what has been described in Section 3.2.1.

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4

Fluid Dynamics in Porous Media: A Boundary Element Approach

Leopold Škerget, Renata Jecl, and Janja Kramer

4.1

Introduction

The main purpose of this chapter is to present a boundary element method as a numerical method for solving problems encountered with flow through porous media. Fluid dynamics in porous media is an important topic in many branches of engineering and science, as well as in many fields of practical interest. It plays a fundamental role in groundwater hydrology, soil mechanics, and petroleum, sanitary and chemical engineering. New computational methods and techniques have allowed us to model and simulate various transport phenomena in a porous medium, and thus a deeper understanding of them is being gained on a perpetual basis. The aim of this chapter is to obtain a numerical solution for the governing equations describing the flow of a viscous incompressible fluid in a porous medium, using an appropriate extension of the boundary element method. The numerical scheme was tested on a natural convection problem within a porous square cavity, where different temperature and concentration values are applied on the vertical walls, as well as in a horizontal porous layer where different temperature and concentration values are applied on the horizontal walls. The results for different governing parameters (Rayleigh number, Darcy number, buoyancy ratio and Lewis number) are presented and compared with published work.

4.1.1

Transport Phenomena in Porous Media

Fluid transport phenomena in a porous medium refer to those processes related to and accompanied by the transport of fluid momentum, mass and heat through the given porous medium. These processes, which are encountered in many different branches of science and technology, are commonly the subject of theoretical treatments which are based on methods traditionally developed in classical fluid dynamics. Natural convection is the most commonly studied transport phenomena in porous media and also a process to which we pay full attention. There have been

several reported studies dealing with natural convection due to thermal buoyancy forces, mainly because of its importance in industrial and technological applications, such as geothermal energy, fibrous insulation, etc. Less attention, however, has been dedicated to so-called double-diffusive problems, where density gradients occur due to the effects of combined temperature and compositional buoyancy. There are some important engineering applications for this phenomenon, such as the transport of moisture in fibrous insulations or grain storage insulations and the dispersion of contaminants through water-saturated soil.

Three main configurations are studied when dealing with double-diffusive natural convection in an enclosure filled with porous media [1,2]:

- temperature and species concentration or their gradients are imposed horizontally along the enclosure, either aiding or opposing each other;
- temperature and species concentration or their gradients are imposed vertically, either aiding or opposing each other; and
- temperature or its gradient is imposed vertically and species concentration or its gradient is imposed horizontally or vice versa.

The present analysis focuses on the use of the boundary element method for solving problems of fluid flows in porous media driven by coupled thermal and solutal buoyancy forces. The Darcy–Brinkman formulation is used for modeling fluid flow in porous media thus enabling a satisfactory nonslip boundary condition on those surfaces that bound the porous medium.

4.1.2

Boundary Element Method for Fluid Dynamics in Porous Media

Fluid flows in porous media have been studied both experimentally and theoretically over recent decades. Different numerical methods have been introduced for obtaining the solutions for some transport phenomena in porous media, e.g. the finite difference method (FDM), finite element method (FEM), finite volume method (FVM), as well as the boundary element method (BEM). The main comparative advantage of the BEM, the application of which requires the given partial differential equation to be mathematically transformed into the equivalent integral equation representation, which is later to be discretized, over the discrete approximative methods, is demonstrated in cases where this procedure results in boundary integral equations only. This turns out to be possible only for potential problems, e.g. inviscid fluid flow, heat conduction, etc. In general, this procedure results in boundary-domain integral equations and, therefore, several techniques have been developed to extend classical BEM. The dual reciprocity boundary element method (DRBEM) represents one of the possibilities for transforming domain integrals into a finite series of boundary integrals (see, for example, [3,4]). The key point of the DRBEM is an approximation of the field in the domain by a set of global approximation functions and the subsequent representation of the domain integrals of these global functions by boundary integrals. The discretization of the domain is only represented by grid points (poles of global approximation functions)

in contrast to FDM meshes. However, the discretization of the geometry and fields on the boundary is piecewise polygonal, which gives this method greater flexibility over the FDMs in coping with boundary quantities. In the DRBEM all calculations reduce to the evaluation of boundary integrals only. Another more recent extension of the BEM is the so-called boundary domain integral method (BDIM) [5–8]. Here, the integral equations are given in terms of variables on the integration boundaries, as well as within the integration domain. This situation arises when we are dealing with strongly nonlinear problems with prevailing domain-based effects, for example diffusion–convection problems. Navier–Stokes equations are commonly used as a framework for the solution of such problems, since they provide a mathematical model of the physical conservation laws of mass, momentum and energy. The velocity–vorticity formulation of these equations results in a computational decoupling of the kinematics and kinetics of the fluid motion from the pressure computation [9]. Since the pressure does not appear explicitly in the field function conservation equations, the difficulty connected with the computation of the boundary pressure values is avoided. The main advantage of the BDIM, as compared to the classical domain-type numerical techniques, is that it offers an effective way of dealing with boundary conditions on the solid walls when solving the vorticity equation. Namely, the boundary vorticity in the BDIM is computed directly from the kinematic part of the computation and not through the use of some approximate formulas. One of the few drawbacks of the BDIM is considerable computing time and memory requirements, but they can be drastically reduced by the use of a subdomain technique [10]. Convection-dominated fluid flows suffer from numerical instabilities. In domain-type numerical techniques upwinding schemes of different orders are used to suppress such instabilities while in the BDIM the problem can be avoided by the use of Green’s functions of the appropriate linear differential operators, which results in a very stable and accurate numerical description of coupled diffusion–convective problems. There are no oscillations in the numerical solutions, which would have to be eliminated by using some artificial techniques, e.g. upwinding, artificial viscosity, as is the case for other approximation methods.

4.2 Governing Equations

Due to the general complexity of the fluid transport process in a porous medium, our work is based on a simplified mathematical model in which it is assumed that:

- the solid phase is homogeneous, nondeformable, and does not interact chemically with respect to the fluid;
- the fluid is single phase and Newtonian; its density does not depend on pressure variation, but only on variation of the temperature;

- the two average temperatures, T_s for the solid phase and T_f for the fluid phase, are identical (the porous medium is in thermodynamic equilibrium), which means the situation is described by a single equation for the average temperature $T = T_s = T_f$;
- no heat sources or sinks exist in the fluid saturated porous medium; thermal radiation and viscous dissipation are negligible;
- porosity and permeability are constant throughout the whole cavity; and
- the density of the fluid depends on temperature and concentration variations and can be described as $\rho = \rho[1 - \beta_T(T - T_0) - \beta_C(C - C_0)]$, where the subscript 0 refers to a reference state, $\beta_T (= -1/\rho[\partial\rho/\partial T]_C)$ is the volumetric thermal expansion coefficient and $\beta_C (= -1/\rho[\partial\rho/\partial C]_T)$ is the volumetric concentration expansion coefficient.

Transport phenomena in the porous media are described using modified Navier-Stokes equations in the form of conservation laws for mass, momentum, energy and species. The equations are written at the macroscopic level, derived by averaging the microscopic equations for a pure fluid over the representative elementary volume. This considers the fact that only a part of the volume expressed with porosity is available for the flow of the fluid and expressed by continuity, momentum, energy and species equations [11]:

$$\frac{\partial v_i}{\partial x_i} = 0 \quad (4.1)$$

$$\frac{1}{\phi} \frac{\partial v_i}{\partial t} + \frac{1}{\phi^2} \frac{\partial v_j v_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + F g_i - \frac{\nu}{K} v_i + \frac{\partial}{\partial x_j} \left(2 \frac{\nu}{\phi} \dot{\epsilon}_{ij} \right) \quad (4.2)$$

$$\frac{\partial}{\partial t} [\phi c_f + (1-\phi)c_s] T + c_f \frac{\partial v_j T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\lambda_e \frac{\partial T}{\partial x_j} \right) \quad (4.3)$$

$$\phi \frac{\partial C}{\partial t} + \frac{\partial v_j C}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D \frac{\partial C}{\partial x_j} \right) \quad (4.4)$$

The parameters used above are: v_i , volume-averaged velocity; x_i , the i th coordinate; ϕ , porosity; t , time; ρ , density; ν , kinematic viscosity; $\partial p/\partial x_i$, the pressure gradient, g_i , gravity; K , permeability of porous media; $\dot{\epsilon}_{ij} (= 1/2(\partial v_i/\partial x_j + \partial v_j/\partial x_i))$, the strain rate tensor; and F , the normalized density difference function, given as $F = (\rho - \rho_0)/\rho_0 = [\beta_T(T - T_0) - \beta_C(C - C_0)]$. Furthermore $C_f = (\rho c)_f$ and $C_s = (\rho c)_s$ are the isobaric specific heat per unit volume for the fluid and solid phases, respectively, T is temperature and λ_e is the effective thermal conductivity of the porous media given as $\lambda_e = \phi \lambda_f + (1 - \phi) \lambda_s$, where λ_f and λ_s are thermal conductivities for the fluid and solid phases, respectively. In Eq. (4.4), C is concentration and D mass diffusivity.

Equation (4.2) is known as the Darcy–Brinkman equation and consists of two viscous terms: the Darcy viscous term (third on the r.h.s.) and the Brinkman viscous term which is analogous to the Laplacian term in Navier–Stokes equations for pure fluid (fourth on the r.h.s.). The Darcy viscous term expresses the viscous resistance or viscous drag force exerted by the solid phase on the flowing fluid at their contact surfaces. A nonslip boundary condition on a surface which bounds the porous media is satisfied by using the additional Brinkman term. There are several situations where it is convenient to use the Brinkman equation, e.g. when one wishes to compare flows in porous media with those in a pure fluid or to investigate convective flows in the context of solidification, where permeability and porosity are variables in space and time. If the included parameter K (the permeability) tends towards infinity ($K \rightarrow \infty$) the Brinkman equation transforms into the classical Navier–Stokes equation for a pure fluid. In contrast, if the permeability tends to zero ($K \rightarrow 0$) the Brinkman term becomes negligible and the equation reduces to a classical Darcy equation [1].

4.3

Boundary Element Method

The BDIM, which is an extension of the classical BEM, is used in order to solve the general set of equations. The discretization of surface and domain is required since boundary and domain integrals are presented in the obtained set of integral equations. Equations (4.1) to (4.4) should be modified in order to use the BDIM. Firstly, the kinematic viscosity in the momentum equation is partitioned into constant and variable parts such as $v = \bar{v} + \tilde{v}$, so the Brinkman term is also divided into two parts, and the equation becomes

$$\frac{\partial v'_i}{\partial t} + \frac{\partial v'_j v'_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + Fg_i - \frac{v\phi}{K} v'_i + \bar{v} \frac{\partial^2 v_i}{\partial x_j \partial x_i} + \frac{\partial}{\partial x_j} (2\tilde{v} \epsilon_{ij}) \quad (4.5)$$

where the term v'_i is now the modified velocity $v'_i = v_i/\phi$. In the same way as kinematic viscosity, the thermal diffusivity a_p , which is defined as $a_p = \lambda_e/c_f$, and the mass diffusivity D are divided into constant and variable parts: $a_p = \bar{a}_p + \tilde{a}_p$, $D = \bar{D} + \tilde{D}$. By including the expression for the heat capacity ratio $\phi + (1 - \phi)c_s/c_f$ in the energy equation, the formulations (4.3) and (4.4) can be rewritten as

$$\frac{\sigma}{\phi} \frac{\partial T}{\partial t} + \frac{\partial v'_j T}{\partial x_j} = \frac{\bar{a}_p}{\phi} \frac{\partial^2 T}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{\tilde{a}_p}{\phi} \frac{\partial T}{\partial x_j} \right) \quad (4.6)$$

$$\frac{\partial C}{\partial t} + \frac{\partial v'_j C}{\partial x_j} = \frac{\bar{D}}{\phi} \frac{\partial^2 C}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{\tilde{D}}{\phi} \frac{\partial C}{\partial x_j} \right) \quad (4.7)$$

4.3.1

Velocity–Vorticity Formulation

In the next step, the above-stated governing equations are transformed by the use of the velocity–vorticity formulation (VVF); consequently the computational scheme is partitioned into its kinematic and kinetic parts [6]. The vorticity vector ω_i is introduced which represents the curl of the velocity field:

$$\omega_i = e_{ijk} \frac{\partial v_k}{\partial x_j} \quad (4.8)$$

where e_{ijk} is the unit permutation tensor. The kinematic part is represented by the elliptic velocity vector equation:

$$\frac{\partial^2 v'_i}{\partial x_j \partial x_j} + e_{ijk} \frac{\partial \omega'_k}{\partial x_j} = 0 \quad (4.9)$$

and kinetics is governed by the vorticity, energy and species transport equation. The vorticity transport equation is obtained as a curl of the Brinkman momentum equation (Eq. 4.5):

$$\frac{\partial \omega'_i}{\partial t} + v'_j \frac{\partial \omega'_i}{\partial x_j} = \bar{v} \frac{\partial^2 \omega'_i}{\partial x_j \partial x_j} + e_{ijk} g_k \frac{\partial F}{\partial x_j} + \omega'_j \frac{\partial v'_i}{\partial x_j} - \frac{v\phi}{K} \omega'_i + \frac{\partial}{\partial x_j} \left(\bar{v} \frac{\partial \omega'_i}{\partial x_j} \right) + \frac{\partial f_{ij}}{\partial x_j} \quad (4.10)$$

where ω'_i is modified vorticity $\omega'_i = \omega_i / \phi$ and f_{ij} any contribution arising on account of nonlinear material properties, given as $f_{ij} = \bar{v}(\bar{\nabla} \times \varepsilon_{ij})$.

The mathematical description of the transport phenomena in fluid flow is completed by providing suitable Dirichlet and Neumann boundary conditions [12], as well as some initial conditions for the energy transport and species transport equations:

$$T = \bar{T} \text{ on } \Gamma_1; \quad \frac{\partial T}{\partial x_j} n_j = \bar{q} \text{ on } \Gamma_2; \quad T = \bar{T}_0 \text{ in } \Omega \quad (4.11)$$

$$C = \bar{C} \text{ on } \Gamma_1; \quad \frac{\partial C}{\partial x_j} n_j = \bar{q} \text{ on } \Gamma_2; \quad C = \bar{C}_0 \text{ in } \Omega \quad (4.12)$$

4.3.2

Boundary Domain Integral Equations

In the present analysis, a two-dimensional problem is considered, so all subsequent equations will be written for the case of planar geometry. The linear elliptic Laplace differential operator can be employed to the velocity equation (Eq. (4.9)):

$$L[\cdot] = \frac{\partial^2 (\cdot)}{\partial x_j \partial x_j} \quad (4.13)$$

and the following relationship for kinematics can be obtained:

$$L[v'_i] + b_i = \frac{\partial^2 v'_i}{\partial x_j \partial x_j} + b_i = 0 \quad (4.14)$$

where b_i is the pseudo-body source term. The integral representation of the velocity vector can be formulated by using the Green theorems for scalar functions or the weighting residuals technique rendering the following vector integral formulation:

$$c(\xi)v'_i(\xi) + \int_{\Gamma} v'_i q^* d\Gamma = \int_{\Gamma} \frac{\partial v'_i}{\partial n} u^* d\Gamma + \int_{\Omega} b_i u^* d\Omega \quad (4.15)$$

where ξ is the source point, u^* is the elliptic Laplace fundamental solution and q^* is its normal derivative, e.g. $q^* = \partial u^* / \partial n$. The fundamental solution u^* is given by the expression

$$u^* = \frac{1}{2\pi} \ln \left(\frac{1}{r(\xi, s)} \right) \quad (4.16)$$

where r is the vector from the source point ξ to the reference field point s . Equating the pseudo-body force as

$$b_i = e_{ij} \frac{\partial \omega'}{\partial x_j} \quad (4.17)$$

we obtain the following integral formulation:

$$c(\xi)v'_i(\xi) + \int_{\Gamma} v'_i q^* d\Gamma = \int_{\Gamma} \frac{\partial v'_i}{\partial n} u^* d\Gamma + e_{ij} \int_{\Omega} \frac{\partial \omega'}{\partial x_j} u^* d\Omega \quad (4.18)$$

The derivative of the vorticity in pseudo-body source terms can be eliminated by using the Gauss divergence theorem. The integral representation of the kinematics is now [13]

$$c(\xi)v'_i(\xi) + \int_{\Gamma} v'_i q^* d\Gamma = \int_{\Gamma} \frac{\partial v'_i}{\partial n} u^* d\Gamma + e_{ij} \int_{\Gamma} \omega' n_j u^* d\Gamma - e_{ij} \int_{\Omega} \omega' q_j^* d\Omega \quad (4.19)$$

By using these expressions for vorticity definition, unit tangent and normal vector, e.g. $\partial v_i / \partial n = \partial v_i / \partial x_j n_j$, $\omega' = e_{ij} \partial v_i / \partial x_j = \partial v_y / \partial x - \partial v_x / \partial y$, $\vec{n} = (n_x, n_y)$ and $\vec{t} = (-n_y, n_x)$ for $i, j = 1, 2$ and applying the continuity Eq. (4.1), the following relationship can be derived:

$$\frac{\partial v'_i}{\partial n} + e_{ij} \omega' n_j = -e_{ij} \frac{\partial v'_j}{\partial t} \quad (4.20)$$

The boundary integrals on the right-hand side of Eq. (4.19) can be rewritten as:

$$c(\xi)v'_i(\xi) + \int_{\Gamma} v'_i q^* d\Gamma = -e_{ij} \int_{\Gamma} \frac{\partial v'_j}{\partial t} u^* d\Gamma - e_{ij} \int_{\Omega} \omega' q_j^* d\Omega \quad (4.21)$$

With further mathematical reformulations and by applying the Gauss theorem, the resulting integral representation can be written as follows:

$$c(\xi)v'_i(\xi) + \int_{\Gamma} v'_i q^* d\Gamma = e_{ij} \int_{\Gamma} v'_j q_t^* d\Gamma - e_{ij} \int_{\Omega} \omega'_j q_j^* d\Omega \quad (4.22)$$

where q_t^* is the tangential derivative of the fundamental solution $q_t^* = \frac{\partial u^*}{\partial t}$, or in the form of the elliptic integral vector formulation:

$$c(\xi)\vec{v}'(\xi) + \int_{\Gamma} \vec{v}' q^* d\Gamma = \int_{\Gamma} (\vec{q}^* \times \vec{n}) \times \vec{v}' d\Gamma + \int_{\Omega} \vec{\omega}' \times \vec{q}^* d\Omega \quad (4.23)$$

The tangential form of Eq. (4.22) can be written as follows:

$$\begin{aligned} c(\xi)\vec{n}(\xi) \times \vec{v}'(\xi) + \vec{n}(\xi) \times \int_{\Gamma} \vec{v}' q^* d\Gamma &= \vec{n}(\xi) \\ &\times \int_{\Gamma} (\vec{q}^* \times \vec{n}) \times \vec{v}' d\Gamma + \vec{n}(\xi) \times \int_{\Omega} \vec{\omega}' \times \vec{q}^* d\Omega \end{aligned} \quad (4.24)$$

in order to obtain an appropriate nonsingular implicit system of equations for unknown boundary vorticity or tangential velocity component values to the boundary [13].

The formulations for the vorticity, temperature and concentration can generally be written as a nonhomogeneous elliptic diffusion–convection equation [8]:

$$\wp \frac{\partial^2 u}{\partial x_j \partial x_j} - \frac{\partial \bar{v}'_j u}{\partial x_j} - \frac{u}{\Delta t} + b_i = 0 \quad (4.25)$$

where u is taken as the vorticity ω' , temperature T and concentration C , respectively, $\wp$ is defined by considering the conservation laws and constitutive hypothesis and is always partitioned as $\wp = \bar{\wp} + \tilde{\wp}$, and b_i is the pseudo-body source term. Since the fundamental solution exists only for steady diffusion–convection partial differential equation (PDE) with constant coefficients, the velocity field is decomposed into an average constant vector $\bar{v}'_i$ and perturbed vector $\tilde{v}'_i$ such that $v'_i = \bar{v}'_i + \tilde{v}'_i$. Thus the following integral formulation can be obtained:

$$c(\xi)u(\xi) + \wp \int_{\Gamma} u q^* d\Gamma = \int_{\Gamma} (\wp q - u \bar{v}'_n) u^* d\Gamma + \int_{\Omega} b_i u^* d\Omega \quad (4.26)$$

where u^* is now the fundamental solution of the steady diffusion–convection PDE with a first-order reaction term [5], in the form of

$$u^* = \frac{1}{2\pi\wp} K_0(\mu r) \exp\left(\frac{\bar{v}'_j r}{2\wp}\right) \quad (4.27)$$

for the plane case. Further, $q^* = \partial u^* / \partial n$ and $q = \partial u / \partial n$ represent the normal derivative of the fundamental solution and suitable field function. Parameter μ is defined as

$$\mu = \sqrt{\left(\frac{\bar{v}'}{2\bar{\rho}}\right)^2 + \frac{k_0}{\bar{\rho}}} = \sqrt{\left(\frac{\bar{v}'}{2\bar{\rho}}\right)^2 + \beta}$$

where $\bar{v}^2 = \bar{v}_j \bar{v}_j$, $\beta = 1/\bar{\rho} \Delta t$, K_0 is the modified Bessel function of the second kind of order 0, and r is the magnitude of the vector from the source to the reference point, i.e. $r = |\mathbf{x}_i(\xi) - \mathbf{x}_i(s)|$. The following integral representations for vorticity, temperature and concentration kinetics are obtained according to Eq. (4.26):

$$\begin{aligned} c(\xi) \omega'(\xi) + \int_{\Gamma} \omega' Q^* d\Gamma &= \frac{1}{\bar{v}} \int_{\Gamma} (\bar{v} q - \omega' \bar{v}'_n + e_{ij} g_j F n_j + f_j n_j) U^* d\Gamma \\ &+ \frac{1}{\bar{v}} \int_{\Omega} (\omega' \bar{v}'_j - e_{ij} g_j F - \bar{v} q_j - f_j) Q_j^* d\Omega + \frac{1}{\bar{v}} \int_{\Omega} \frac{\bar{v} \phi}{K} \omega' U^* d\Omega \\ &+ \frac{1}{\bar{v} \Delta t} \int_{\Omega} \omega'_{F-1} U^* d\Omega \end{aligned} \quad (4.28)$$

$$\begin{aligned} c(\xi) T(\xi) + \int_{\Gamma} T Q^* d\Gamma &= \frac{\phi}{\sigma \bar{a}_p} \int_{\Gamma} \left(\frac{\sigma \bar{a}_p}{\phi} q - T \bar{v}'_n \right) U^* d\Gamma \\ &- \frac{\phi}{\sigma \bar{a}_p} \int_{\Omega} \left(\frac{\sigma \bar{a}_p}{\phi} q_j - T \bar{v}'_j \right) Q_j^* d\Omega + \frac{\phi}{\sigma \bar{a}_p \Delta t} \int_{\Omega} T_{F-1} U^* d\Omega \end{aligned} \quad (4.29)$$

$$\begin{aligned} c(\xi) C(\xi) + \int_{\Gamma} C Q^* d\Gamma &= \frac{\phi}{\bar{D}} \int_{\Gamma} \left(\frac{\bar{D}}{\phi} q - C \bar{v}'_n \right) U^* d\Gamma \\ &- \frac{\phi}{\bar{D}} \int_{\Omega} \left(\frac{\bar{D}}{\phi} q_j - C \bar{v}'_j \right) Q_j^* d\Omega + \frac{\phi}{\bar{D} \Delta t} \int_{\Omega} C_{F-1} U^* d\Omega \end{aligned} \quad (4.30)$$

where $Q^* = \partial U^* / \partial n$ represents a normal and $Q_j^* = \partial U^* / \partial x_j$ a space derivative of the modified elliptic diffusion-convective solution U^* defined as $U^* = \bar{v} u^*$ in the momentum equation, $U^* = \bar{a}_p / \phi u^*$ in the energy equation and $U^* = \bar{D} / \phi u^*$ in the species equation. Further, $q = \partial u / \partial n$ represents a normal and $q_j = \partial u / \partial x_j$ a space derivative of the field function (vorticity, temperature, concentration).

4.3.3

Discretized Boundary Domain Integral Equations

For an approximate numerical solution, the integral equations are written in a discretized manner, where the integrals over boundary and domain are approximated by the sum of integrals over all boundary elements and internal cells, respectively. The variation of field functions within each boundary element or internal cell is

approximated by the use of appropriate interpolation polynomials [14]. After applying the discretized integral equations to the boundary and internal nodes, the implicit matrix systems can be obtained, firstly for the kinematic computational part:

$$[H]\{v'_i\} = e_{ij}[H_t]\{v'_j\} - e_{ij}[D_j]\{\omega'\} \quad (4.31)$$

Furthermore, we obtain the implicit systems for the vorticity kinetics

$$\begin{aligned} [H]\{\omega'\} = & \frac{1}{V}[G]\{vq - \omega'v'_n + e_{ij}g_jFn_j + f_jn_j\} \\ & + \frac{1}{V}[D_j]\{\omega'v'_j - e_{ij}g_jF - \tilde{v}q_j - f_j\} + \frac{1}{V}[B]\left\{\frac{v\phi}{K}\omega'\right\} + \frac{1}{V\Delta t}[B]\{\omega'_{F-1}\} \end{aligned} \quad (4.32)$$

then the heat energy kinetics

$$[H]\{T\} = \frac{\phi}{\sigma\bar{a}_p}[G]\left\{\frac{\sigma\bar{a}_p}{\phi}q - T\tilde{v}'_n\right\} - \frac{\phi}{\sigma\bar{a}_p}[D_j]\left\{\frac{\sigma\bar{a}_p}{\phi}q_j - T\tilde{v}'_j\right\} + \frac{\phi}{\sigma\bar{a}_p\Delta t}[B]\{T\}_{F-1} \quad (4.33)$$

and finally the species kinetics

$$[H]\{C\} = \frac{\phi}{D}[G]\left\{\frac{D}{\phi}q - C\tilde{v}'_n\right\} - \frac{\phi}{D}[D_j]\left\{\frac{\tilde{D}}{\phi}q_j - C\tilde{v}'_j\right\} + \frac{\phi}{D\Delta t}[B]\{C\}_{F-1} \quad (4.34)$$

In the above equations, the matrices $[H]$, $[H_t]$, $[G]$, $[D_j]$ and $[B]$ are the influence matrices composed of those integrals which took over the individual boundary elements and internal cells. This system of discretized equations is solved by coupling these kinetic and kinematic equations and considering the corresponding boundary and initial conditions. Since the implicit set of equations is written simultaneously for all boundary and internal nodes, this procedure results in a very large and fully populated system matrix, influenced by diffusion and convection. The consequence of this approach is a very stable and accurate numerical scheme with substantial computer time and memory demands. The subdomain technique is used to improve the economics of the computation, where the entire computational domain is partitioned into subdomains to which the same described numerical procedure can be applied. The final system of equations for the entire domain is then obtained by adding the sets of equations for each subdomain and considering the compatibility and equilibrium conditions between their interfaces, resulting in a sparser matrix system, suitable for solving by using iterative techniques. In the present case, each subdomain consists of four discontinuous 3-node quadratic boundary elements and one 9-node corner continuous quadratic internal cell [6].

4.3.4

Solution Procedure

The obtained set of discretized Eqs. (4.31) to (4.34) is solved by coupling the kinetic and kinematic equations. In this way, the solenoidality of the velocity field for an

arbitrary vorticity distribution is ensured. The following numerical algorithm has to be performed in order to obtain a final solution:

1. Start with some initial values for the vorticity distribution.
2. Kinematic computational part:
 - solve implicit set for boundary vorticity values (Eq. 4.31),
 - determine new domain velocity values.
3. Energy kinetic computation part:
 - solve implicit set for boundary and domain values (Eq. 4.33).
4. Species kinetic computation part:
 - solve implicit set for boundary and domain values (Eq. 4.34).
5. Vorticity kinetic computational part:
 - solve implicit set for unknown boundary vorticity flux and internal domain vorticity values (Eq. 4.32).
6. Relax new values and check the convergence. If the convergence criterion is satisfied, then stop; otherwise go to step 2.

4.4

Numerical Examples

4.4.1

Double-Diffusive Natural Convection in Vertical Cavity

The most commonly studied geometry of simultaneous heat and mass transfer in porous media is a rectangular cavity where vertical walls are maintained at different temperatures and solute concentrations. The first reported comprehensive numerical study of this problem is given in [15]. Numerical results for overall heat and mass transfer through porous cavity are presented using a Darcy model and compared with scale analysis for several parameters, which govern natural convection. The same phenomena are considered for the case of constant temperature and solute concentration gradients applied on the vertical walls in [16]. Different modeling is done because of a more frequent occurrence of practical conditions that approach the constant heat and mass fluxes descriptions, rather than the constant temperature and concentration model. This model is also more suitable for obtaining analytical solutions for overall heat and mass transfer calculations. The same problem using a Darcy model is considered in [17,18] for cases of cooperative and opposing thermal and solutal buoyancy forces. The results of numerical, analytical and scale analysis are reported. Double-diffusive natural convection with opposing buoyancy effects in a porous medium is studied in [19]. The Darcy model is again used for simulating the fluid flow. A comprehensive numerical study of double-diffusive natural convection in a porous cavity using the Darcy–Brinkman formulation is reported in [20]. It was the first work using the Darcy–Brinkman model for studying double-diffusive natural convection which is also suitable for studying convection in the context of solidification, where permeability and porosity are not constant in space and time. The results

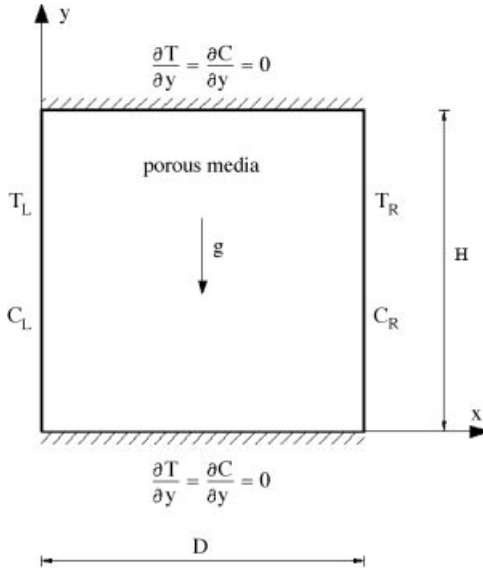


Figure 4.1 Geometry of a two-dimensional cavity with boundary conditions.

are divided into analyses of mass and heat transfer, respectively. The influence of main dimensionless parameters is considered. A generalized non-Darcy approach as used for analyzing double-diffusive natural convective flow is presented in [21]. The non-Darcy effects on the flow are investigated and the influence of non-Darcy parameters as Darcy number and porosity on heat and mass transfer are observed.

The system under consideration is a two-dimensional (2D) square cavity with side length L , filled with a fluid saturated porous medium. The solid phase is assumed to be homogeneous, isotropic and nondeformable, the fluid is Newtonian and in thermal equilibrium with the solid phase. Furthermore, the flow is incompressible, laminar, 2D and in steady state, which satisfies the Boussinesq approximation. Porosity and permeability are assumed to be constant throughout the whole cavity. The vertical walls are subjected to different temperatures and concentrations (T_L and C_L at the left wall, T_R and C_R at the right wall) while the horizontal walls are adiabatic and impermeable (Figure 4.1).

The validity of the proposed numerical scheme is practically discussed over a large range of parameters which govern the phenomena of natural convection:

- porosity ϕ ,
- permeability of the porous media K ,
- Darcy number $Da = (1/\phi)(K/L^2)$,
- modified (porous) Rayleigh number $Ra^* = RaDa\lambda$, where $Ra_T = g\beta_T D^3 \Delta T / \nu \alpha_f$ is the Rayleigh number for the pure fluid,
- heat capacity ratio $\sigma = \phi + (1 - \phi)c_s/c_f$,
- Lewis number $Le = Sc/Pr$, where Sc is the Schmidt number, $Sc = \nu/D$, and Pr is the Prandtl number, $Pr = \nu/\alpha$, and
- buoyancy coefficient $N = \beta_C \Delta C / \beta_T \Delta T$.

In the above notations L is the length of the cavity side, λ is the heat conductivity ratio $\lambda = a_f/a_p$, where a_f is the heat conductivity of the fluid and a_p is the heat conductivity of the porous media, β_T and β_C are coefficients of thermal and concentration expansion, respectively, and ΔT and ΔC are temperature and concentration differences between the left and right walls.

Most of the double-diffusive natural convection research inside a porous medium is limited to the Darcy regime, which is governed by the modified Rayleigh number Ra^* , the Lewis number Le and the buoyancy coefficient N . In this present study, attention is focused on a non-Darcy parameter, Darcy number, which represents the effect of the additional Brinkman viscous term in the momentum equation.

Because of the present study's simplicity, the values of conductivity ratio and heat capacity ratio have been taken as $\lambda = \sigma = 1$, and the porosity $\phi = 0.5$. A nonuniform computational 20×20 mesh was used with a ratio between the longest and shortest elements of $r = 6$. Time-steps ranging from $\Delta t = 10^{16}$ (steady state) to $\Delta t = 10^{-3}$ were employed, and the convergence criterion determined as $\varepsilon = 5 \times 10^{-6}$. The results for total heat and mass transfer through the porous cavity are given by the values of the Nusselt and Sherwood numbers, which are defined as:

$$Nu = - \int_0^1 \left(\frac{\partial T}{\partial x} \right)_{x=0} dy, \quad Sh = - \int_0^1 \left(\frac{\partial C}{\partial x} \right)_{x=0} dy \quad (4.21)$$

The effects of the Darcy, Rayleigh and Lewis numbers and the buoyancy coefficient on the overall heat and mass transfer were studied. The influence of the Brinkman term due to increasing viscous forces ($Da = 10^{-1}$ – 10^{-7}) was analyzed. The presented results have been compared with those obtained using the Darcy model (corresponding to a very small value of Darcy number, in our case $Da = 10^{-7}$).

In order to firstly test the accuracy of the presented numerical algorithm, the results for purely thermal natural convection (corresponding to a buoyancy coefficient $N = 0$) are presented and compared with those reported in the literature. The average values for the Nusselt number regarding parameters $Ra^* = 100$, $Ra^* = 500$, $Le = 1$ and $Da = 10^{-1}$ – 10^{-7} are given in Table 4.1 and compared with work [8,22] which deals with a natural convection due to thermal buoyancy forces using the Darcy–Brinkman model.

Table 4.1 Average Nusselt number Nu for $Le = 1$ and $N = 0$.

Da		10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$Ra^* = 100$	Present results	1.08	1.70	2.43	2.83	2.99	3.12	3.13
	[8]	1.086	1.695	2.414	2.847	2.995	–	–
	[22]	–	1.70	2.41	2.84	3.02	3.06	3.09
$Ra^* = 500$	Present results	1.704	3.20	5.35	7.32	8.38	8.70	8.81
	[8]	1.681	3.145	5.235	7.185	8.428	–	–
	[22]	–	3.30	5.42	7.35	8.41	8.72	8.84

Table 4.2 Average Nusselt and Sherwood numbers for $Da = 10^{-7}$, $Le = 10$, $N = 0$.

Ra^*		100	200
Nu	Present results	3.13	5.06
	[15]	3.27	5.61
	[20]	3.11	4.96
Sh	Present results	14.26	22.25
	[15]	15.61	23.23
	[20]	13.25	19.86

The overall heat transfer is the same as the overall mass transfer, because the value of the Lewis number is $Le = 1$ and buoyancy coefficient $N = 0$. Therefore, the values of the Nusselt and Sherwood numbers are identical. It is evident from Table 4.1 that with any decrease in the Darcy number, the value of the Nusselt number increases, which is a consequence of the additional Brinkman term in the momentum equation. At higher values for the Darcy number, the effect of viscous forces is significant and slows down the convective motion in porous media, which results in lower heat transfer. When the Darcy number decreases, the viscous effect becomes smaller, and at $Da = 10^{-7}$ it can be said to be negligible. It can be seen that the obtained results are in good agreement with those reference solutions available in the literature.

Table 4.2 presents the results for average mass transfer due to purely thermal natural convection ($N = 0$) for $Le = 10$. The solutal buoyancy force is still absent, so mass transfer is induced by thermally driven flow. The mass transfer is higher than the corresponding heat transfer because of higher values for the Lewis number ($Le > 1$). The Lewis number is increased by the Schmidt number (at the fixed Prandtl number), which directly reduces the solutal boundary layer's thickness, and leads to a higher Sherwood number [20]. The results are now compared with those proposed by Trevisan and Bejan [15] and Goyeau *et al.* [20]. Both studies deal with double-diffusive natural convection, the first one using a Darcy model and the second one a Darcy–Brinkman model. There is a discrepancy between the published results, which is commented on in [20]; however, the present results are in better agreement with the solutions in [20], than those obtained using the Darcy model.

The effects of those viscous forces accounted for in the additional Brinkman term on the flow in the porous cavity are illustrated in Figures 4.2 to 4.4. The velocity, temperature and concentration field for a modified Rayleigh number $Ra^* = 100$, Lewis number $Le = 10$, buoyancy coefficient $N = 1$ and different Darcy numbers $Da = 10^{-1}$, 10^{-3} , 10^{-7} are represented.

It can be observed from the velocity field at small values of Darcy number (Figure 4.2c) that streamlines are closely spaced near those solid boundaries where the fluid velocity reaches its maximum ($Da \rightarrow 0$, Darcy law). The Darcy number in this case is small enough for any viscous effect on the boundaries to become negligible. With any increase in Darcy number the streamlines near the solid boundaries are sparsely spaced (Figure 4.2a and b), as a result of higher viscous forces that become more important and slow down the fluid motion near the solid walls.

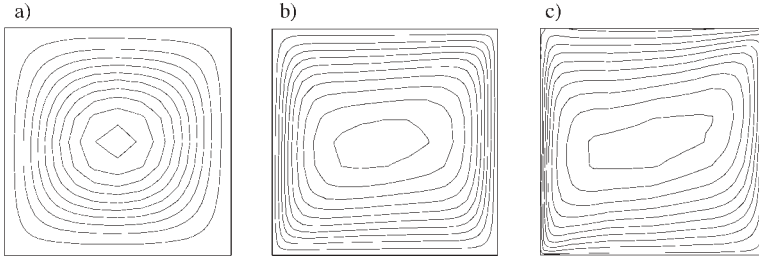


Figure 4.2 Streamlines for $Ra^* = 100$, $Le = 10$, $N = 1$ and (a) $Da = 10^{-1}$, (b) $Da = 10^{-3}$, (c) $Da = 10^{-7}$.

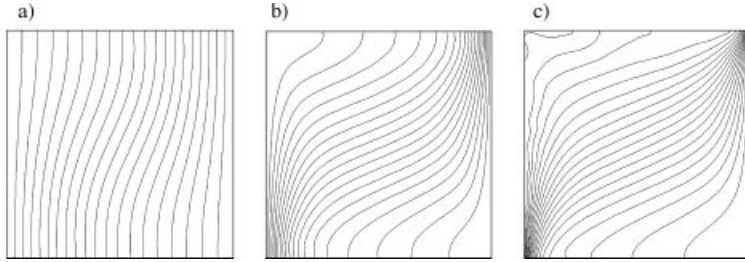


Figure 4.3 Isotherms for $Ra^* = 100$, $Le = 10$, $N = 1$ and (a) $Da = 10^{-1}$, (b) $Da = 10^{-3}$, (c) $Da = 10^{-7}$.

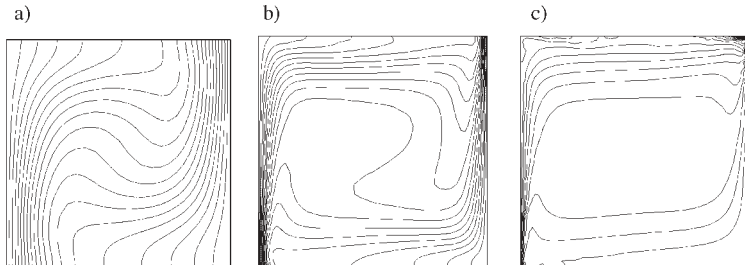


Figure 4.4 Isoconcentrations for $Ra^* = 100$, $Le = 10$, $N = 1$ and (a) $Da = 10^{-1}$, (b) $Da = 10^{-3}$, (c) $Da = 10^{-7}$.

The effect of the additional viscous term is also obvious on the simulation of the temperature field (Figure 4.3). The heat transfer through the cavity is strong at smaller values of the Darcy number (Figure 4.3c). When the Darcy number increases and the viscous effect becomes more important, the isotherms become more linear and the convective motion through the cavity slows down (Figure 4.3a and b).

The concentration field (Figure 4.4) presents the classic stratified structures of the natural convective flows. As in the two previous cases, here the influence of the

Table 4.3 Average Nusselt and Sherwood numbers for $Ra = 100$, $Le = 10$, $N = 1$, $Da = 10^{-1}$, 10^{-3} , 10^{-7} .

Da	10^{-1}	10^{-3}	10^{-7}
<i>Nu</i>	1.04	2.58	3.75
<i>Sh</i>	2.37	10.08	21.40

additional viscous term can also be identified. At higher values of the Darcy number, when the influence of the Brinkman term is important, the concentration gradients at the solid boundaries are smaller than in the case where $Da \rightarrow 0$. The mass transfer through the porous cavity is considerably higher at lower values of Da .

Finally, the results for buoyancy coefficients $N > 0$ are given in Table 4.3 where the average values of the Nusselt and Sherwood numbers for $N = 1$, $Ra^* = 100$, $Le = 10$, and different Darcy numbers are presented.

The buoyancy ratio characterizes the relative magnitude of the thermal and solutal buoyancy force and, generally, increases the overall heat and mass transfer. It is evident from Table 4.3 that the Nusselt and Sherwood numbers increase with any decrease in the Darcy number, as also shown for the pure thermal cases ($N = 0$). In comparison with the results for $N = 0$, the overall heat and mass transfers are now higher because of the cooperating buoyancy forces. The convective heat transport of overall heat transfer increases with any increase in N . The global buoyancy term in the momentum equation increases with the buoyancy ratio and enhances the flow velocity and overall heat transfer. The mass transfer also increases with the stronger influence of the solutal buoyancy force.

The results for $Ra^* = 100$, $Da = 10^{-1}$, $Le = 1$, $Le = 10$ and various buoyancy numbers $N = -1, 0, 1, 2, 5, 10$ are calculated in Table 4.4.

The results in Table 4.4 show that the Nusselt number decreases with any increase in the Lewis number Le ; in contrast, the values of the Sherwood numbers are higher with any increases in Le and N . Negative values for the buoyancy coefficient N imply an opposing configuration of thermal and solutal buoyancy effects. In the case where $N = -1$ the thermal and solutal buoyancy forces cancel each other, so the heat and mass transfer are governed by diffusion (the values of the Nusselt and Sherwood numbers are $Nu = Sh = 1.0$) as also observed in [15], for the case of a Darcy model.

Table 4.4 Average Nusselt and Sherwood numbers for $Ra^* = 100$, $Le = 1$, $Da = 10^{-1}$, $N = -1, 0, 1, 2, 5, 10$.

N		-1	0	1	2	5	10
<i>Le</i> = 1	<i>Nu</i>	1.00	1.08	1.26	1.43	1.81	2.21
	<i>Sh</i>	1.00	1.08	1.26	1.43	1.81	2.21
<i>Le</i> = 10	<i>Nu</i>	1.00	1.00	1.07	1.09	1.15	1.19
	<i>Sh</i>	1.00	1.08	2.66	2.95	3.56	4.25

4.4.2

Double-Diffusive Natural Convection in a Horizontal Porous Layer

The convective flow in a horizontal porous layer is possible above the critical Rayleigh number. In the case of double-diffusive convection, where the density differences are a result of combined temperature and concentration gradients, the critical Rayleigh number is a function of the Darcy number Da , Lewis number Le and buoyancy coefficient N [23]. In vertical cavities maintained at horizontal temperature and concentration gradients, the flow in the cavity is always unicellular. In the case of a horizontal porous layer, where the temperature and concentration differences are imposed on the horizontal walls, the flow structure becomes multicellular and is also called a Rayleigh–Benard flow structure [24].

Most of the studies regarding double-diffusive convection or thermohaline convection (the case where the constituent is salt) in a horizontal porous layer are focused on the problem of convective instability. There are many studies dealing with the onset of convection on the basis of the linear stability theory [25,26] or nonlinear perturbation theory [27]. In these studies, the critical Rayleigh numbers for the onset of convective flows are predicted. The theoretical and numerical study of heat and mass transfer affected by a high Rayleigh number Benard convection in a porous layer heated from below can be found in [28]. The numerical results and a scale analysis of the flow in a porous medium are presented, where the buoyancy effect is due entirely to temperature gradients.

Some further numerical results for a double-diffusive convection in a horizontal porous layer with two opposing buoyancy sources can be found in [29]. The influence of the governing parameters (Rayleigh number, Lewis number, buoyancy ratio) on the overall heat and mass transfer is discussed for the case of a square cavity (aspect ratio equals 1). Double-diffusive convection in a horizontal layer with some numerical results is also discussed in [30]. In this study, the critical values of Rayleigh numbers for the onset of convective motion are predicted on the basis of nonlinear parallel flow approximation.

All the numerical results mentioned above are obtained on the basis of the Darcy flow model, which is more convenient for porous media with low permeability. The Brinkman extended Darcy model, which accounts for friction due to macroscopic shear, is more appropriate when describing fluid flows in a porous matrix, when the inertia effects are negligible. It was used in [23] to investigate the onset and development of double-diffusive convection in a horizontal porous layer with uniform heat and mass fluxes specified at the horizontal boundaries. The obtained analytical solution is compared to some numerical results obtained for different values of Ra , N , Le and Da .

In our case, the system under consideration is a horizontal layer of width D and height H , filled with homogenous, nondeformable porous media, which is fully saturated with Newtonian fluid (Figure 4.5).

The horizontal walls are subjected to different temperature and concentration values (T_B , C_B at the bottom boundary and T_U , C_U at the upper boundary), while the vertical walls are adiabatic and impermeable. The fluid, saturating the porous media,

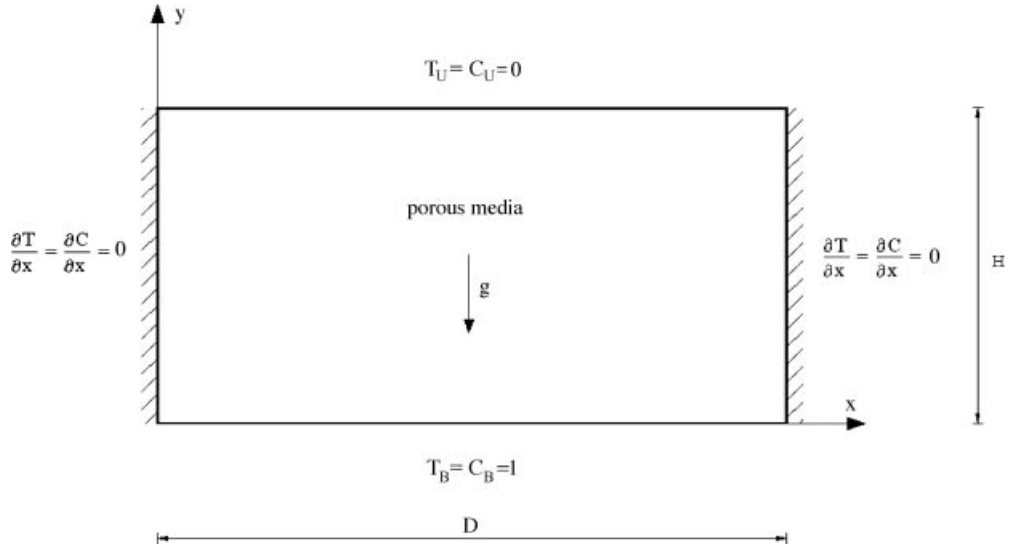


Figure 4.5 Geometry of the problem and boundary conditions.

is modeled as a Boussinesq incompressible fluid, where the density depends only on temperature and concentration variations: $\rho = \rho_0(1 - \beta_T(T - T_0) - \beta_C(C - C_0))$. Parameters β_T and β_C are volumetric thermal and concentration expansion coefficients. The numerical results for heat and mass transfer induced by double-diffusive natural convection in a horizontal porous layer subjected to vertical gradients of temperature and concentration are presented.

The governing parameters of a problem are:

- porosity ϕ ,
- Darcy number $Da = K/\phi H_2$,
- aspect ratio $A = D/H$,
- modified (porous) thermal Rayleigh number $Ra = Kg\beta_T\Delta TH/\alpha\nu$, where β_T is the thermal expansion coefficient, α the thermal diffusivity and ν the viscosity,
- Lewis number $Le = \alpha/D$, and
- buoyancy ratio $N = \beta_C\Delta C/\beta_T\Delta T$,

where K is the permeability, D and H are the width and height of the layer, respectively, g is the gravity, ΔT and ΔC the temperature and concentration differences between the upper and bottom boundaries, α the thermal diffusivity and D the mass diffusivity. For an aspect ratio $A = 1$, a nonuniform computational 20×20 mesh was used with a ratio between the longest and shortest elements of $r = 6$, and for $A = 2$ and 4, 20×10 subdomains were used. Time-steps ranging from $\Delta t = 10^{16}$ (steady state) to $\Delta t = 10^{-4}$ were employed, and the convergence criterion determined as $\varepsilon = 5 \times 10^{-6}$ for all cases.

Table 4.5 Comparison of results with numerical experiments reported in the literature for $A = 1$.

	Nu		Sh	
	This study	[29]	This study	[29]
$Ra = 600, Le = 1, N = 0$	7.01	6.6	7.01	—
$Ra = 100, Le = 10, N = 0.2$	2.48	2.4	10.00	—
$Ra = 100, Le = 30, N = 0.2$	2.50	2.5	14.80	15

It should be noted that in the case of $N = 0$, the buoyancy effect is due entirely to temperature gradients. The mass transfer in this case is due to temperature field and concentration differences between the horizontal boundaries. In the case of positive values for buoyancy ratio ($N > 0$), the thermal and solutal buoyancy forces aid each other (aiding convection) and for negative values of buoyancy ratio ($N < 0$) the solutal and thermal effects have opposite tendencies (opposing convection).

The obtained numerical model was tested for different values for governing parameters. The results for total heat and mass transfer through the horizontal layer are given by the values of Nusselt (Nu) and Sherwood numbers (Sh). Furthermore, some simulations of the temperature and concentration fields are presented.

The validation of the code was accomplished by comparison with some published numerical experiments. It should be noted that there are not many published studies giving numerical results for the described problem.

Table 4.5 presents some results for $A = 1$, $Da = 10^{-5}$ and different Rayleigh and Lewis numbers and buoyancy ratio.

The values of overall heat and mass transfer are compared to the published results, where the numerical calculations based on the Darcy model are obtained [29]. The first result is for the case of $Ra = 600$, $Le = 1$ and $N = 0$ which means that only the thermal buoyancy force is present. The overall heat and mass transfers which are presented by Nu and Sh are identical. The other two cases are for a Rayleigh number of 100, a buoyancy ratio 0.2 and Lewis numbers of 10 and 30. In this case, both the thermal and solutal buoyancy forces are present and aid each other. The values of the Sherwood numbers are now higher than those of the Nusselt numbers, which is a result of a higher Lewis number. The presented results are in agreement with published ones.

Table 4.6 presents the influence of the Darcy number. The governing parameters for this case are: an aspect ratio $A = 4$, a Rayleigh number $Ra = 300$, a Lewis number $Le = 1$ and a buoyancy ratio $N = -2$.

Table 4.6 Nu and Sh numbers for different values of Da with $A = 4$, $Ra = 300$, $Le = 1$, $N = -2$.

Da	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
Nu	1.00	2.05	2.82	3.12	3.50
Sh	1.00	1.02	1.04	1.05	1.06

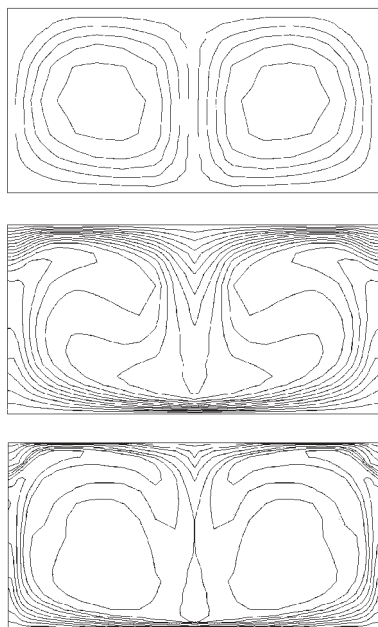


Figure 4.6 Streamlines, isotherms and isoconcentrations in a horizontal layer for $Ra = 2500$, $Da = 10^{-2}$, $Le = 10$, $N = 0$, $A = 2$.

The negative sign for buoyancy ratio indicates that the thermal and solutal buoyancy forces are opposed to each other. From Table 4.6 it is evident that with any decrease in the Darcy number the value of the Nusselt number increases. In the cases where the Lewis number decreases, $Le \rightarrow 0$, the values of the Sherwood number tend to unity ($Sh \rightarrow 1$), which implies that the mass transfer is dominated by diffusion. The same conclusions are also published in [23]. A direct comparison of results is impossible, because of the different governing parameters (porosity, aspect ratio) in both studies.

In the case of $Da = 10^{-1}$ the values of the Nusselt and Sherwood numbers are equal to 1, which means that both heat and mass transfer are governed by diffusion. The Rayleigh number is beyond the critical value required for the beginning of convective motion. The relationship between the critical Rayleigh number and the Darcy number is given in [23] and states that the values of the critical Rayleigh number increase in line with the Darcy number.

The velocity, temperature and concentration fields for $Ra = 2500$, $Da = 10^{-2}$, $Le = 10$, $N = 0$, $A = 2$ are presented in Figure 4.6. Because the value of the buoyancy ratio equals 0, the buoyancy effect is due entirely to temperature gradients. The concentration field, in this case, is a result of the flow driven by the temperature gradients and the imposed concentration difference between the upper and bottom boundaries.

The flow in the horizontal layer where $A = 2$ becomes multicellular (with two cells) as is obvious from Figure 4.6. The flow consists of rising hot fluid in the center

of the layer and colder fluid sinking along the vertical walls. In the center of the domain, higher solute concentration is found than along the adiabatic and impermeable side walls. Thin temperature and composition boundary layers are evident at the top and bottom walls.

4.5

Conclusion

A numerical approach, based on the BDIM, which is an extension of the BEM, has been applied for the solutions of the transport equations in porous media. The modified Navier–Stokes equations, Brinkman-extended Darcy formulation with the inertial term included, have been employed to describe the fluid motion in porous media. The porous media are saturated with a viscous, incompressible fluid. A velocity–vorticity formulation of the governing equations is adopted, resulting in the computational decoupling of the kinematics and kinetics of the fluid motion from the pressure computation. Since the pressure does not appear explicitly in the field function conservation equations, the difficulty connected with the computation of boundary pressure values is avoided. The proposed numerical procedure is applied to the case of natural convection in a porous cavity saturated with a Newtonian fluid with different temperature and concentration values on its vertical walls, and in a porous layer where the horizontal walls are subjected to different values of temperature and concentration, for different values of the modified Rayleigh number, Darcy number, Lewis number and buoyancy coefficient. It can be stated that the BDIM, extended in a way that also enables investigation of the fluid transport phenomena in a porous medium, appears to possess the potential to become a very powerful alternative to existing numerical methods, e.g. finite differences or finite elements, as a means for obtaining solutions to the most complex systems of nonlinear partial differential equations, when attacking some unsolved problems in engineering practice.

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5

Analytical Methods for Heat Conduction in Composites and Porous Media

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5.1

Introduction

The goal of this chapter is to describe analytical methods applied to the study of steady heat conduction in various types of composites and porous media. We present several analytical formulas for the effective (macroscopic) conductivity tensor which are deduced by using different approaches based on the recent results in the theory of partial differential equations and complex analysis. The study of effective characteristics has recently become a separate subject with its own philosophy and machinery. Composites and porous media differ by geometry and by the type of physical problems that appear. For composites, the most popular are problems of conductivity, elasticity, elastoplasticity and thermoelasticity (e.g. Refs. [1–4]), but for porous media, problems of fluid mechanics are mostly studied (e.g. Refs. [5–9]).

The analytical approach to the study of heat conduction allows us to unify partly the theory of the effective thermal properties in composite materials and porous media. In the present chapter, pure steady conductivity problems are considered when the filler of pores (fluid or gas) is static. Such problems are benchmarks of heat and mass transfer problems of the mechanics of porous media [5,6,10].

The main attention throughout this chapter will be paid to *analytic* or *constructive*, or *closed form solutions* to the above mentioned problems. Different interpretations can be given to such a notion. For us to get an analytical solution means to find the formula which contains a finite set of elementary and special functions, compositions, integrals, derivatives and even series. Besides, all objects in such a formula have to have a precise meaning (for instance, the type of the convergence of integrals and series should be described). Last, the domains of parameters, as well as all functions, integrals, etc., have to be explicitly determined. It will also be shown also that they (or their intersections, if necessary) are nonempty. This approach is slightly nontraditional. In classic books, it is supposed that series do not form closed form solutions, but special functions do. It leads to certain misunderstandings since not

all special functions have integral representations. We suppose that our meaning of a closed form solution could give a way to work efficiently with the mathematical object involved in the solution formulas.

The above meaning of analytic solutions is very close to the sense of solutions obtained by certain numerical methods. To avoid misunderstandings we will distinguish between (pure) analytic solutions and those obtained by using certain analytic numerical procedure. The latter will be called *approximate analytic solutions*.

Among the numerical methods which can be called approximate analytical methods we have to point out the collocation method and its modifications as developed and applied to the study of composites by Kolodziej and co-workers [11–13], the finite element method presented in other chapters of this book, the integral equation method, in the form developed, for example, by Lifanov [14,15], as well as the successive approximation method and methods of decomposition, in particular, Schwarz's alternating method (all applied in the study of composites in Ref. [16]). Despite the method of truncation for infinite linear algebraic systems can be effective in numerical computations, one can hardly accept that this method yields a "closed form solution" as is frequently declared.

In this review, the main attention is paid to analytically exact and approximate formulas for the effective conductivity tensor. Other important questions as bounds [17], homogenization [1,2,17–20], coupled heat and mass transfer [5,6,10] can be found in the cited works.

5.2

Mathematical Models for Heat Conduction

5.2.1

General

Consider the Euclidian space $\mathbb{R}^M$ as a space of the spatial variable $\mathbf{x} = (x_1, x_2, \dots, x_M)$. Usually $M = 3$. Sometimes due to the symmetry of the problem under discussion it is convenient to take $M = 2$ or $M = 1$, making corresponding changes in the equations. Let D be a domain occupied by the conducting material (composite or porous media). One of the most important objects in the mathematical theory of steady heat conduction is *the temperature distribution* $T(\mathbf{x})$ and *the heat flux* $\mathbf{q}(\mathbf{x})$. In physics, temperature is the measure of the energy possessed by particles (molecules, electrons, etc.) per unit volume of the material. The heat flux is the heat transfer rate (in unit of time) per unit volume. Below, the dimensions of the basic variables can be taken in SI units. The unit for temperature is the kelvin K , for heat flux it is $Jm^{-2}s^{-1}$, for conductivity it is $Wm^{-1}K^{-1}$, where J is the joule, m is the meter, s is the second, W is the watt.

From a mathematical point of view $T(\mathbf{x})$ is a scalar field depending on the variable $\mathbf{x} \in \mathbb{R}^M$, $\mathbf{q}(\mathbf{x}) = (q_1(\mathbf{x}), q_2(\mathbf{x}), q_3(\mathbf{x}))$ is a vector field. The equations representing dependence of the flux $\mathbf{q}(\mathbf{x})$ on the temperature $T(\mathbf{x})$ are called (the heat transfer) *constitutive*

relations. In the linear case the constitutive relation for conducting material has the form of Fourier's law (e.g. Ref. [4,5,8,10])

$$\mathbf{q} = -\Lambda \nabla T \quad (5.1)$$

where ∇T is the gradient of $T(\mathbf{x})$ and Λ is a tensor. In Cartesian coordinates $\nabla T = \left(\frac{\partial T}{\partial x_1}, \frac{\partial T}{\partial x_2}, \frac{\partial T}{\partial x_3} \right)$.

The constitutive relation (5.1) means a (local) proportionality of the flux and the gradient of temperature distribution. In the linear case, the proportionality coefficient Λ depends solely on the spatial variable $\mathbf{x}$. It is the measure of the heat conduction of the solid phase. For locally isotropic media, $\Lambda = \lambda \mathbf{I}$, where $\mathbf{I}$ is the identity tensor. Then, λ is called *the local thermal conductivity* or simply *the conductivity*. The thermal conductivity is considered as a scalar positive function $\lambda = \lambda(\mathbf{x})$ for locally isotropic materials and as a tensor function for locally anisotropic materials which in Cartesian coordinates has the form of the symmetric positively defined matrix:

$$\Lambda = \Lambda(\mathbf{x}) = \begin{pmatrix} \lambda_{11}(\mathbf{x}) & \lambda_{21}(\mathbf{x}) & \lambda_{31}(\mathbf{x}) \\ \lambda_{12}(\mathbf{x}) & \lambda_{22}(\mathbf{x}) & \lambda_{23}(\mathbf{x}) \\ \lambda_{13}(\mathbf{x}) & \lambda_{23}(\mathbf{x}) & \lambda_{33}(\mathbf{x}) \end{pmatrix} \quad (5.2)$$

For Λ depending on the temperature, i.e., $\Lambda = \Lambda(\mathbf{x}, T)$ we deal with *nonlinear heat conduction*.

Sometimes the thermal resistance r is introduced as $r = \lambda^{-1}$ ($R = \Lambda^{-1}$), where the power -1 denotes the reciprocal whenever λ is a function (the matrix inverse whenever Λ is a matrix).

Assuming the presence of sources and sinks with intensity $f(\mathbf{x})$, we get the following relation $\nabla \cdot \mathbf{q} = f$ in D . If a medium does not contain sources or sinks, the heat flux satisfies the so-called *free divergence equation*:

$$\nabla \cdot \mathbf{q} = 0 \quad (5.3)$$

or in Cartesian coordinates $\frac{\partial q_1}{\partial x_1} + \frac{\partial q_2}{\partial x_2} + \frac{\partial q_3}{\partial x_3} = 0$.

Substituting (5.3) into (5.1), we obtain the elliptic equation [21]:

$$\nabla \cdot (\Lambda \nabla T) = 0 \quad (5.4)$$

Laplace Equation In the case of isotropic homogeneous material, the conductivity $\lambda(\mathbf{x})$ is a constant. Then, (5.4) becomes the *Laplace equation* [21]:

$$\nabla^2 T = 0 \quad (5.5)$$

i.e., T is a harmonic function in D . The constitutive relation (5.1) means in this case that the flux $\mathbf{q}(\mathbf{x})$ has a potential (in other words, the vector field $\mathbf{q}(\mathbf{x})$ is a potential one, or the considered physical system is conservative; e.g. Refs. [22,23]).

Geometry The domain D occupied by the medium is supposed to be an arbitrary open set in $\mathbb{R}^M$, $M = 3$ (or $M = 2$). Usually it is supposed that D consists of a finite or denumerable collection of connected components. One of the components Ω , called the matrix or host material, contains other components as inclusions or pores.

If the boundary surfaces (or curves) are simple and smooth, then two continuous families of normal vectors can be chosen. Each one generates an orientation on the surface (on the curve). Most common is to choose an orientation generated by outward unit normal vectors $\mathbf{n}$ to $\partial\Omega$, understanding such an orientation as positive and an opposite orientation as a negative one. Such a definition can be extended to domains with piecewise smooth boundaries.

The level of smoothness of the boundary can also be prescribed. For simplicity, it is usually supposed that $\partial\Omega$ consists of piecewise Lyapunov's (or $C^{1,\alpha}$ ($0 < \alpha \leq 1$)) surfaces or curves. It means that they have a tangent plane (a tangent line) everywhere besides a finite number of smooth curves on a surface (finite number of points on a curve), and the corresponding field of normal vectors is Hölder continuous with respect to the spatial variable on a surface (on a curve). Therefore, corner (wedge) points can arise on the boundary surfaces (curves). It usually brings additional difficulties to attack problems (e.g., Refs. [24–26]).

Sometimes it is important to model the conducting medium by a certain infinite domain. Different compactifications can be applied in this case. For instance, in a 2D situation ($M = 2$) it is convenient to understand ∞ as the unique point extension of the complex plane $\mathbb{C}$ (i.e. as a north pole on the Riemann sphere $S^2 = \hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$) (e.g., Ref. [27]). In this case, the point ∞ can be either boundary point of a domain D or its internal point (on the sphere $\hat{\mathbb{C}}$). Another possibility is to consider several infinite points.

Spaces Looking for a classical solution, we need to prescribe certain smoothness of these solutions on the boundary. Let us recall definitions of the most standard spaces of smooth and piecewise smooth functions on a connected subset $X \subset \mathbb{R}^M$ (in particular, on each connected component of X).

It is said that the family $\mathcal{C}(X) = \{f : X \rightarrow \mathbb{C}(\mathbb{R}) : f \text{ is continuous on } X\}$ forms a linear space of *continuous functions*. For X being either a closed surface or a closed curve, $\mathcal{C}(X)$ becomes a Banach space under the norm $\|f\|_c = \sup_{\mathbf{x} \in X} |f(\mathbf{x})|$. The spaces $\mathcal{H}^\alpha(X)$ containing *Hölder-continuous functions* are introduced by the following condition:

$$\mathcal{H}^\alpha(X) = \{f \in \mathcal{C}(X) : \exists C > 0, \quad |f(\mathbf{x}_1) - f(\mathbf{x}_2)| < C|\mathbf{x}_1 - \mathbf{x}_2|^\alpha, \\ \forall \mathbf{x}_1, \mathbf{x}_2 \in X\}, 0 < \alpha \leq 1$$

(here $|\mathbf{x}_1 - \mathbf{x}_2|$ means the Euclidean distance between two points of $X \in \mathbb{R}^M$). These spaces are called *Hölder spaces*. They are linear subspaces of $\mathcal{C}(X)$ (the following notations for them are also commonly used: $Lip_\alpha(X)$, $C^{0,\alpha}$). Again for X being either a closed surface or a closed curve, $\mathcal{H}^\alpha(X)$ becomes a Banach space

with the following norm:

$$\|f\|_{\alpha} = \|f\|_C + \sup_{\mathbf{x}_1, \mathbf{x}_2 \in X, \mathbf{x}_1 \neq \mathbf{x}_2} \frac{\|f(\mathbf{x}_1) - f(\mathbf{x}_2)\|}{|\mathbf{x}_1 - \mathbf{x}_2|^{\alpha}} =: \|f\|_C + h(f; \alpha)$$

For X being a nonclosed piecewise smooth surface or curve one can introduce *weighted Hölder spaces*:

$$\mathcal{H}^{\alpha}(X; \rho) = \{f : \exists f_0, \quad f(\mathbf{x}) = f_0(\mathbf{x})\rho(\mathbf{x}), \quad f_0 \in \mathcal{H}^{\alpha}(X)\}$$

with a given weight function ρ (for instance, $\rho(\mathbf{x}) = \prod_{l=1}^n |\mathbf{x} - \mathbf{x}_l|^{\beta_l}$, where $\beta_l \in \mathbb{R}$).

To introduce the spaces of differentiable functions in $\mathbb{R}^M$, it is convenient to use the notion of multi-index. Let, for example, $\mathbf{x} = (x_1, x_2, x_3) \in X \subset \mathbb{R}^3$, $f : X \rightarrow \mathbb{C}(\mathbb{R})$. Denote by $\partial_j f = \frac{\partial f}{\partial x_j}$ the derivative of f with respect to j -th variable. The vector $k = (k_1, k_2, k_3) \in \mathbb{Z}_+^3$ is called multi-index, and $|k| = k_1 + k_2 + k_3$ denotes its length. By definition, k -th (partial) derivative of f is equal to $\partial^k f = \frac{\partial^{|k|} f}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$. Then, $\mathcal{C}^m(X)$, $m \in \mathbb{N}$, is a space of all functions $f : X \rightarrow \mathbb{C}(\mathbb{R})$ such that $f(\mathbf{x})$ and $\partial^k f, |k| \leq m$, are continuous on X . We have to note that for X being a smooth surface or a smooth curve the derivatives can be taken only in the tangent direction to X .

The collection of *Schauder spaces* is defined in the following way ($m \in \mathbb{N}$, $0 < \alpha \leq 1$):

$$\mathcal{C}^{m, \alpha}(X) = \{f \in \mathcal{C}^m(X) : \exists C > 0, \quad |\partial^k f(\mathbf{x}_1) - \partial^k f(\mathbf{x}_2)| < C |\mathbf{x}_1 - \mathbf{x}_2|^{\alpha}, \\ \forall \mathbf{x}_1, \mathbf{x}_2 \in X, \quad |k| = m\}$$

They are Banach spaces for X being a smooth surface or a smooth curve under the following norms:

$$\|f\|_{m, \alpha} = \sum_{|k|=0}^m \|\partial^k f\|_C + \sum_{|k|=m} h(\partial^k f; \alpha)$$

Finally, the collection of all *infinitely differentiable functions* is denoted by $\mathcal{C}^{\infty}(X)$:

$$\mathcal{C}^{\infty}(X) = \{f \in \mathcal{C}(X) : \forall k \in \mathbb{Z}_+^3, \forall \mathbf{x} \in X, \exists \partial^k f(\mathbf{x})\}$$

It should be noted that we can consider $\mathbb{R}^2$ to be isometric to $\mathbb{C}$. Thus, in this case in all the above definitions the partial derivatives can be replaced by the derivatives with respect to complex variable. These definitions are stronger than those with partial derivatives with respect to two real variables [27].

Let Γ be a simple closed curve in $\mathbb{C}$, $X = \text{int } \Gamma$. The set of all continuous functions $\mathcal{C}(\Gamma)$ analytically extended into X is denoted by $\mathcal{C}_A(\Gamma)$ (or $\mathcal{C}_A(X)$). It is a Banach space under supremum norm on $\text{cl } X$. Analogous definitions (under corresponding norms in $\text{cl } X$) are used for the spaces $\mathcal{C}_A^{m, \alpha}(\Gamma) = \mathcal{C}_A^{m, \alpha}(X)$, $\mathcal{C}_A^{\infty}(\Gamma) = \mathcal{C}_A^{\infty}(X)$.

In many problems of mathematical physics it is not sufficient to deal only with the classical solutions corresponding to differential equations. One of the most suitable generalizations of the above introduced spaces are the so-called *Sobolev spaces* (e.g., Ref. [28]). The main idea in the construction of these spaces is the use of the notion of *weak derivatives*.

Let $X \subset \mathbb{R}^M$ be an open connected set. We denote by $L_p(X)$, $1 \leq p < \infty$, the set of all (Lebesgue-) measurable functions $f : X \rightarrow \mathbb{C}(\mathbb{R})$ such that

$$\|f\|_p = \left(\int_X |f(\mathbf{x})|^p d\mathbf{x} \right)^{1/p} < \infty$$

It is a Banach space with respect to the norm $\|f\|_p$. It is said that $X' \subset X \subset \mathbb{R}^M$ is a strictly interior subdomain of X , if $\bar{X}' \subset X$ (the corresponding notation is $X' \subset\subset X$). The space $L_{p,loc}(X)$, $1 \leq p < \infty$, is the set of all (Lebesgue-) measurable functions $f : X \rightarrow \mathbb{C}(\mathbb{R})$ such that $\int_{X'} |f(x)|^p d\mathbf{x} < \infty$ for any bounded strictly interior domain $X' \subset\subset X$. Denote also by $C_0^\infty(X)$ the class of all compactly supported infinitely differentiable functions $f : X \rightarrow \mathbb{C}(\mathbb{R})$.

Let now k be a multi-index, the functions $f, g \in L_{1,loc}(X)$, and the following relation be satisfied:

$$\int_X f(\mathbf{x}) \partial^k \eta(\mathbf{x}) d\mathbf{x} = (-1)^{|k|} \int_X g(\mathbf{x}) \eta(\mathbf{x}) d\mathbf{x}$$

for all functions $\eta \in C_0^\infty(X)$. Then, g is called the *weak derivative* of f . It is denoted by the same symbol as before, namely $g = \partial^k f$.

The Sobolev space $W^{s,p}(X)$, $1 \leq p < \infty$, $s \in \mathbb{Z}_+$, is the set of all functions $f \in L_p(X)$ for which there exist weak derivatives $\partial^k f$ for any k , $|k| < s$, such that $\partial^k f \in L_p(X)$, $\forall |k| \leq s$. Endowed by the norm $\|f\|_{s,p,X} = \sum_{|k| \leq s} \|\partial^k f\|_p$, $W^{s,p}(X)$ becomes a Banach space. In the special case $p = 2$, the space $W^{s,2}(X)$ is denoted by $H^s(X)$. This space is a Hilbert space with the inner product defined by the relation

$$\langle f, g \rangle_{s,X} = \sum_{|k| \leq s} \langle \partial^k f, \partial^k g \rangle_{L_2(X)} = \sum_{|k| \leq s} \int_X \partial^k f(\mathbf{x}) \overline{\partial^k g(\mathbf{x})} d\mathbf{x}$$

The set $C_0^\infty(X)$ is a dense subset of $H^1(\mathbb{R}^M)$. If $X \neq \mathbb{R}^M$ then the closure of $C_0^\infty(X)$ in H^1 -norm is a subspace of $H^1(X)$ denoted by $H_0^1(X)$.

The set of all linear continuous functional $H_0^1(X)$ with respect to inner form in $H_0^1(X)$:

$$\langle f, g \rangle_{1,X} = \left(\int_X f(\mathbf{x}) \overline{g(\mathbf{x})} d\mathbf{x} + \sum_{|k|=1} \int_X \partial^k f(\mathbf{x}) \overline{\partial^k g(\mathbf{x})} d\mathbf{x} \right)$$

is denoted by $H^{-1}(X)$.

Let Q be a parallelepiped in $\mathbb{R}^M$, $M=2,3$, then $\mathcal{C}_{A,per}^{m,\alpha}(\partial Q) = \mathcal{C}_{A,per}^{m,\alpha}(Q)$, $\mathcal{C}_{A,per}^\infty(\partial Q) = \mathcal{C}_{A,per}^\infty(Q)$, $W_{per}^{s,p}(Q)$, $H_{per}^s(Q)$ are subspaces of $\mathcal{C}_A^{m,\alpha}(Q)$, $\mathcal{C}_A^\infty(Q)$, $W^{s,p}(Q)$, $H^s(Q)$, respectively, containing those functions which possess periodic extension from the set Q to the space $\mathbb{R}^M$.

5.2.2

Boundary Value Problems

Let us present different types of boundary value problem for heat conduction in composites and porous media (i.e. boundary value problems for equations (5.4) and (5.5)).

To be more precise, we formulate these problems in the case of composites consisting of the matrix (which is a multiply connected domain Ω in $\mathbb{R}^2$ with outer boundary curve Γ) and of n inclusions D_k , $k=1, \dots, n$, encircled by smooth closed surfaces (curves) $L_k = \partial D_k$. It is convenient to use the notation $\Lambda(\mathbf{x})$ for the conductivity tensor for the material occupied by the host domain Ω , and $\Lambda_k(\mathbf{x})$, $k=1, \dots, n$, for the conductivity tensors for the material occupied by the corresponding inclusions (see Section 5.2.1).

We suppose that either $M=3$ or $M=2$, just by making corresponding remarks when these situations differ essentially. According to the above presented description of the orientation on the boundary of Ω , we will denote by $T(\mathbf{t})$ the boundary values of the temperature distribution on Γ , and the boundary limits on L_k of the temperature from the domain Ω and domains D_k by $T^+(\mathbf{t})$, $T_k^-(\mathbf{t})$, respectively:

$$\begin{aligned} T(\mathbf{t}) &= \lim_{\mathbf{x} \rightarrow \mathbf{t} \in \Gamma, \mathbf{x} \in \Omega} T(\mathbf{x}); \quad T^+(\mathbf{t}) = \lim_{\mathbf{x} \rightarrow \mathbf{t} \in L_k, \mathbf{x} \in \Omega} T(\mathbf{x}), \quad k=1, \dots, n; \\ T_k^-(\mathbf{t}) &= \lim_{\mathbf{x} \rightarrow \mathbf{t} \in L_k, \mathbf{x} \in D_k} T(\mathbf{x}) \end{aligned}$$

The given temperature distribution $f(\mathbf{t})$ on the outer boundary Γ leads to the Dirichlet condition on Γ :

$$T(\mathbf{t}) = f(\mathbf{t}), \quad \mathbf{t} \in \Gamma \quad (5.6)$$

If the outer boundary constitutes the ideal thermal isolator (i.e. there is no heat exchange between the composite and the medium outside of it), then we arrive at the homogeneous Neumann condition

$$\frac{\partial T}{\partial \mathbf{n}}(\mathbf{t}) = 0, \quad \mathbf{t} \in \Gamma \quad (5.7)$$

If there is heat transfer through the outer boundary when the normal heat flux $\mathbf{q} \cdot \mathbf{n}$ is known at the outer surface, then condition (5.7) should be replaced by a more complicated one (see Eq. (5.1))

$$\Lambda \nabla T \cdot \mathbf{n}(\mathbf{t}) = g(\mathbf{t}), \quad \mathbf{t} \in \Gamma \quad (5.8)$$

Here, $\Lambda \nabla T$ denotes that the matrix Λ is multiplied by the vector $\nabla \Lambda$. Further, the scalar product of the vectors $\Lambda \nabla T$ and $\mathbf{n}$ is calculated.

Instead of Eq. (5.8), the heat transfer satisfying Newton's law can be considered at the boundary

$$\lambda \frac{\partial T}{\partial \mathbf{n}}(\mathbf{t}) + \gamma T(\mathbf{t}) = h(\mathbf{t}), \quad \mathbf{t} \in \Gamma \quad (5.9)$$

It is also called the third type boundary value problem.

5.2.3

Conjugation Problem

Other types of condition arise on internal components of the boundary of Ω , i.e. on the matrix–inclusions (host–pores) interface. The most natural are continuity of the temperature and of the heat flux. For simplicity, hereafter the scalar conductivity is considered. Then, they have the following form

$$T^+(\mathbf{t}) = T_k^-(\mathbf{t}), \quad \lambda \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) = \lambda_k \frac{\partial T_k^-}{\partial \mathbf{n}}(\mathbf{t}), \quad \mathbf{t} \in L_k (k = 1, \dots, n) \quad (5.10)$$

They are known as the *perfect contact* or *transmission* conditions. It is also natural to assume that the temperature distribution and the normal heat flux have jumps along a part of the matrix–inclusions interface. In this case, conditions (5.10) have the following form:

$$T^+(\mathbf{t}) - T_k^-(\mathbf{t}) = h_k(\mathbf{t}), \quad \lambda \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) - \lambda_k \frac{\partial T_k^-}{\partial \mathbf{n}}(\mathbf{t}) = g_k(\mathbf{t}), \quad \mathbf{t} \in L_k (k = 1, \dots, n) \quad (5.11)$$

where h_k, g_k are given functions on L_k .

If at least a part of the matrix–inclusions interface consists of poorly conducting material then we have to replace the first series of the above conditions by a more complicated one, namely, we have the following problem:

$$\lambda \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) + \gamma_k (T^+(\mathbf{t}) - T_k^-(\mathbf{t})) = 0, \quad \lambda \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) = \lambda_k \frac{\partial T_k^-}{\partial \mathbf{n}}(\mathbf{t}), \quad \mathbf{t} \in L_k (k = 1, \dots, n) \quad (5.12)$$

The coefficients γ_k^{-1} introduced in Eq. (5.12) is known as the Kapitza resistances [3,29]. The limit cases $\gamma_k = 0$, and $\gamma_k = \infty$ were discussed in Ref. [16].

A special problem can be also considered, namely with the boundary conditions given on the exterior boundary and the domains D_k occupied by an ideal conductor ($\lambda_k = \infty$). In this case, we arrive at the modified Dirichlet problem [30]

$$T(\mathbf{t}) = t_k, \quad \mathbf{t} \in L_k \quad (5.13)$$

where t_k are undetermined constants which have to be found in the solution to the problem.

5.2.4

Complex Potentials

The aim of this subsection is to rewrite equations as well as boundary value problems for heat conduction in composites (or in porous media) in terms of complex analysis. Thus, we have studied here only the two-dimensional situation ($M=2$) considering the corresponding domains as domains on the complex plane $\mathbb{C}$. In this case, it is supposed that the heat flux is spreading in a direction orthogonal to the cylinder in which parallel cylindrical inclusions are implemented. The base of the cylinder is a multiply connected domain Ω , and the bases of the inclusions are domains D_k . There is also another statement of the 2D problem when a thick plate with isolated sides is considered.

First, we consider the limit cases when Ω is occupied by a conducting material and on the boundary of which one of the boundary conditions (5.6), (5.8) and (5.9) are given. Consider the Dirichlet problem (5.6). It is known that each harmonic function in a simply connected domain is the real part of a complex potential. If a function $T(x, y)$ is harmonic in a multiply connected domain Ω then it can be expressed as

$$T(z) = \operatorname{Re} \left[\Phi(z) + \sum_{k=1}^n A_k \ln(z - z_k) \right], \quad z = x_1 + ix_2 \in \Omega \quad (5.14)$$

according to the decomposition theorem [16]. Here, the function $\Phi(z)$ is analytic and single-valued in Ω , and A_k are real numbers. If we assume that $\infty \in \Omega$, D_k ($k = 1, 2, \dots, n$) are connected components of the complement of Ω to $\mathbb{C}$, and z_k are points in D_k , then the connectivity of Ω is equal to $n - 1$ and

$$\sum_{k=1}^n A_k = 0 \quad (5.15)$$

Substituting $T(z)$ from Eq. (5.14) in Eq. (5.6), we arrive at the boundary value problem with respect to $\Phi(z)$. The constants A_k have also to be determined. One can find a discussion of this problem for multiply connected domains in Ref. [30] and a complete solution to this problem for any circular multiply connected domain in Ref. [16]. A similar argument can be applied to the problems (5.7) and (5.9).

Consider now the modified Dirichlet problem (5.13). In this case, instead of (5.14) we have $T(z) = \operatorname{Re} \Phi(z)$. However, the undetermined constants t_k are included in the boundary condition

$$\operatorname{Re} \Phi(t) = t_k, \quad t \in L_k \quad (k = 1, 2, \dots, n)$$

We also suppose (again for simplicity) that the materials inside matrix and inclusions are isotropic and homogeneous, which means the constancy of conductivity coefficients $\lambda, \lambda_k, k = 1, \dots, n$. Therefore, the temperature T is a harmonic function in the domains Ω and $D_k, k = 1, \dots, n$ (i.e. satisfies in these domains the Laplace equation (5.5)).

Let T , and T_k be temperature distributions in Ω and D_k , $k = 1, \dots, n$, respectively, continuously differentiable up to the boundaries of these domains satisfying Eq. (5.5). Suppose that the perfect contact relations (5.10) are valid on each curve $L_k = \partial D_k$, $k = 1, \dots, n$. Then, one can introduce functions

$$\begin{aligned} \varphi(z) = T(z) + iV(z), \quad z \in \Omega, \quad \varphi_k(z) = \frac{\lambda + \lambda_k}{2\lambda} (T_k(z) + iV_k(z)), \\ z \in D_k, \quad k = 1, \dots, n \end{aligned} \quad (5.16)$$

which are analytic in Ω , D_k , respectively, continuously differentiable in the closures of the considered domains. In fact (e.g. Ref. [22]), the function $\varphi(z)$ is in general a multivalued analytic function since Ω is a multiply connected domain. But in our case, $T(z)$ possesses [31] a unique harmonic extension up to the function, harmonic in a simply connected domain $D = \Omega \cup \bigcup_{k=1}^n L_k \cup \bigcup_{k=1}^n D_k$ due to the first relations in Eq. (5.10).

Therefore, due to the uniqueness of analytic continuation $\varphi(z)$ is a single-valued analytic function in Ω as the restriction of the corresponding function defined on D .

In order to represent the boundary conditions (5.10) in the complex form, we write the normal and tangent derivatives on a fixed curve L_k :

$$\frac{\partial}{\partial \mathbf{n}} = n_1 \frac{\partial}{\partial x_1} + n_2 \frac{\partial}{\partial x_2}, \quad \frac{\partial}{\partial \mathbf{s}} = -n_2 \frac{\partial}{\partial x_1} + n_1 \frac{\partial}{\partial x_2} \quad (5.17)$$

where the normal vector $\mathbf{n}$ is identified with the complex number, $\mathbf{n} = n_1 + in_2$, the tangent vector $\mathbf{s} = n_2 - in_1$, and $z = x_1 + ix_2$. By applying the second operator of Eq. (5.17) to the first condition of Eq. (5.10), we obtain

$$-n_2 \frac{\partial T^+}{\partial x_1} + n_1 \frac{\partial T^+}{\partial x_2} = -n_2 \frac{\partial T_k^-}{\partial x_1} + n_1 \frac{\partial T_k^-}{\partial x_2} \quad (5.18)$$

The second condition of Eq. (5.10) can be rewritten in a similar way

$$\lambda n_1 \frac{\partial T^+}{\partial x_1} + \lambda n_2 \frac{\partial T^+}{\partial x_2} = \lambda_k n_1 \frac{\partial T_k^-}{\partial x_1} + \lambda_k n_2 \frac{\partial T_k^-}{\partial x_2} \quad (5.19)$$

We introduce new complex potentials in the domains Ω and D_k , respectively,

$$\Psi = \frac{\partial \varphi}{\partial z} = \frac{\partial T}{\partial x_1} - i \frac{\partial T}{\partial x_2}, \quad \Psi_k = \frac{\lambda_k + \lambda}{2\lambda} \left(\frac{\partial \varphi_k}{\partial z} \right) = \frac{\lambda_k + \lambda}{2\lambda} \left(\frac{\partial T_k}{\partial x_1} - i \frac{\partial T_k}{\partial x_2} \right) \quad (5.20)$$

Then, substituting these relations into Eqs. (5.18) and (5.19) and excluding $\overline{\Psi^+}$, we arrive at the following conjugation condition:

$$\Psi^+(t) = \Psi_k^-(t) + \rho_k \overline{\mathbf{n}^2 \Psi_k^-(t)}, \quad t \in L_k \quad (5.21)$$

where

$$\rho_k = \frac{\lambda_k - \lambda}{\lambda_k + \lambda} \quad (5.22)$$

is a contrast parameter introduced by Bergman [32,33]. Integrating Eq. (5.21) along L_k with constant of integration equal to zero [16], we obtain the following boundary value problem for analytic functions in a multiply connected domain, namely, for the complex potentials φ, φ_k , $k = 1, \dots, n$:

$$\varphi^+(t) = \varphi_k^-(t) - \rho_k \overline{\varphi_k^-(t)}, \quad t \in L_k \quad (5.23)$$

This problem is a special case of so-called $\mathbb{R}$ -linear conjugation problem (Markushovich's problem) (see Refs. [34,35] for the description of qualitative results concerning the solvability of $\mathbb{R}$ -linear conjugation problem with arbitrary coefficients).

If at least one of the first conditions in Eq. (5.10) is replaced by a non-zero jump condition, i.e. we have Eq. (5.11), then one can proceed in a similar way as before. We introduce the complex potentials by formulas (5.16). If h_k are smooth enough, e.g. $h_k \in C^{1,\alpha}(L_k)$, then one can find (single-valued) analytic in D_k functions $h_k^-(z)$ satisfying the following boundary conditions (the so-called Schwarz boundary value problem):

$$\operatorname{Re} h_k^-(t) = h_k(t), \quad t \in L_k \quad (5.24)$$

Then, the first conditions of Eq. (5.11) can be rewritten in the form $T^+(t) - \tilde{T}_k^-(t) = 0$, $t \in L_k$, $k = 1, \dots, n$, where $\tilde{T}_k^-(z) = T_k^-(z) + \operatorname{Re} h_k^-(z)$, $z \in D_k$. A similar argument can be applied to the second condition (5.11). Thus, the last relations give the single-valuedness of the potential $\varphi^+(z)$ in Ω . Then by using the above introduced complex potentials (5.16), we deduce that the only difference is that at least one of the Eqs. (5.18) is in this case inhomogeneous. As a result, we will have the following boundary value problem with non-zero inhomogeneous term $c_k(t)$ on at least one curve L_k :

$$\varphi^+(t) = \varphi_k^-(t) - \rho_k \overline{\varphi_k^-(t)} + c_k(t), \quad t \in L_k \quad (5.25)$$

Exact calculation of the inhomogeneous term can be easily done. It does not have much influence on further analysis.

Application of the same arguments to Eq. (5.12) yields an $\mathbb{R}$ -linear conjugation problem with derivatives. Let us assume for simplicity that the inclusions are circular cylinders, i.e. $D_k = \{z \in \mathbb{C} : |z - a_k| < r_k\}$, $k = 1, \dots, n$. Then, the problem (5.12) becomes

$$\varphi^+(t) = \varphi_k^-(t) - \rho_k \overline{\varphi_k^-(t)} + \mu_k (t - a_k) (\varphi_k^-)'(t) + \mu_k \frac{r_k^2}{t - a_k} \overline{(\varphi_k^-)'(t)}, \quad |t - a_k| = r_k \quad (5.26)$$

where $\mu_k = \frac{1 + \rho_k}{2r_k \gamma_k}$.

Finally, we have to rewrite the boundary conditions on the outer boundary Γ in the complex form too. The simplest is to reformulate the Dirichlet condition (5.6). We

first solve the outer Schwarz boundary value problem

$$\operatorname{Re} f_0(t) = f(t), \quad t \in \Gamma \quad (5.27)$$

with respect to the function $f_0(z)$ analytic outside of the whole domain $D = \Omega \bigcup_{k=1}^n L_k \bigcup_{k=1}^n D_k$, i.e. in *ext* D . Then by introducing an auxiliary unknown function $\varphi_0(z)$ analytic in *ext* D , $\varphi_0(\infty) = 0$ and using the same complex potential $\varphi(z)$ for Ω , we rewrite Eq. (5.6) in the form of $\mathbb{R}$ -linear conjugation problem:

$$\varphi^+(t) = \varphi_0(t) - \overline{\varphi_0(t)} + f_0(t), \quad t \in \Gamma \quad (5.28)$$

A similar approach is used for the Neumann problem (5.7) (for complex potential ψ) [16].

Problems (5.10) and (5.11) were discussed for arbitrary multiply connected domains in Ref. [30] and solved explicitly for any multiply connected domain in Ref. [16].

5.2.5

Periodic Problems

Boundary value problems for harmonic and analytic functions discussed in the previous sections are also stated in classes of periodic functions. As it follows from the theory of homogenization [17,18,20], such problems are the basis for rigorous definition of the effective conductivity tensor. In the present section, we state periodic problems.

Consider a lattice $\mathcal{Q}$ which is defined by three fundamental translation vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. Hereafter, we consider orthogonal lattices, i.e. the vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ generate an orthogonal system of coordinates. For definiteness, we put $\mathbf{a} = (\alpha, 0, 0)$, $\mathbf{b} = (0, \beta, 0)$, $\mathbf{c} = (0, 0, \gamma)$. Let $\mathbf{m} = (m_1, m_2, m_3)$ denote vectors with integers components. Introduce the zero-th cell (representative cell) $\mathcal{Q} \equiv \mathcal{Q}_0 := \{\mathbf{x} = (x_1, x_2, x_3) : -\alpha/2 < x_1 < \alpha/2, -\beta/2 < x_2 < \beta/2, -\gamma/2 < x_3 < \gamma/2\}$. The lattice $\mathcal{Q}$ generates the cells $\mathcal{Q}_{\mathbf{m}} := \{\mathbf{x} \in \mathbb{R}^3 : (x_1 - \alpha m_1, x_2 - \beta m_2, x_3 - \gamma m_3) \in \mathcal{Q}\}$. Without loss of generality, it is assumed that the volume of $\mathcal{Q}$ is equal to unity, i.e. $|\mathcal{Q}| = \alpha\beta\gamma = 1$. Consider mutually disjoint domains D_k ($k = 1, 2, \dots, n$) lying in the zero-th cell $\mathcal{Q}$. Let D be the complement of the closure of all D_k to $\mathcal{Q}$.

Let a constant external gradient (q_1, q_2, q_3) be applied to the material. Then, the temperature distribution satisfies the conjugation condition (5.10) and the quasi-periodicity relations with respect to the lattice $\mathcal{Q}$:

$$\begin{aligned} T(x_1 + \alpha, x_2, x_3) - T(x_1, x_2, x_3) &= q_1 \\ T(x_1, x_2 + \beta, x_3) - T(x_1, x_2, x_3) &= q_2 \\ T(x_1, x_2, x_3 + \gamma) - T(x_1, x_2, x_3) &= q_3 \end{aligned} \quad (5.29)$$

Theorem 5.2.1 [17,20] *The problem (5.10), (5.29) with fixed q_1 , q_2 and q_3 has a unique solution in $H^1(Q)$ up to an arbitrary additive real constant.*

In this subsection, the condition of the perfect contact (5.10) is considered. In a similar way, other boundary and conjugation problems can be stated. Frequently, instead of the quasi-periodicity conditions (5.29) boundary conditions are introduced for symmetric problems as follows. Let the cell Q be symmetric with respect to the coordinate axes, i.e. the inclusions are symmetrically located in Q . Let the external gradient $(q_1, 0, 0)$ be applied to the periodic material. Then, the the heat flux is symmetric with respect to the planes $x_2 = \beta/2 + m$ and $x_3 = \gamma/2 + m$, where $m = 0, \pm 1, \pm 2, \dots$. In particular, this symmetry yields the Neumann condition:

$$\frac{\partial T}{\partial x_2}(x_1, \pm\beta/2, x_3) = 0, \quad \frac{\partial T}{\partial x_3}(x_1, x_2, \pm\gamma/2) = 0 \quad (5.30)$$

The first quasi-periodicity conditions (5.29) for the temperature distribution yield the periodicity conditions for $\frac{\partial T}{\partial x_1}$ on the planes $x_1 = \pm\alpha/2$. Then, T is a constant on $x_1 = \pm\alpha/2$ and one can take the Dirichlet conditions:

$$T(\pm\alpha/2, x_2, x_3) = \pm q_1/2 \quad (5.31)$$

Therefore, the quasi-periodic problems (5.10), (5.29) becomes the mixed problem (5.10), (5.30), (5.31) for the domain Q . Such an approach is applied in Section 5.5.

Following Section 5.2.4, consider 2D quasi-periodic problems by the method of complex potential. In this case, it is convenient to express the fundamental translation vectors by the complex numbers α and $i\beta = i/\alpha$. The problem (5.10), (5.29) becomes the $\mathbb{R}$ -linear conjugation problem (5.23) with the quasi-periodicity conditions

$$\varphi(z + \alpha) - \varphi(z) = q_1 + id_1, \quad \varphi(z + i\alpha^{-1}) - \varphi(z) = q_2 + id_2 \quad (5.32)$$

where q_1 and q_2 are given real constants, d_1 and d_2 are undetermined real constants which should be found. The function $\varphi(z)$ is analytic in D , D_k , continuously differentiable in the closure of the considered domains.

The problems (5.10) and (5.32) can be considered as an $\mathbb{R}$ -linear conjugation problem on the torus represented by the cell Q . It can also be considered as an $\mathbb{R}$ -linear conjugation problem for an infinitely connected domain bounded by $\partial D_k + m$ ($m = m_1\alpha + im_2\alpha^{-1}$, and m_1 and m_2 run over integers).

Along similar lines, the periodic $\mathbb{R}$ -linear conjugation problem can be stated in the form (5.21). Additionally, $\psi(z)$ satisfies the periodicity conditions

$$\psi(z + \alpha) - \psi(z) = 0, \quad \psi(z + i\alpha^{-1}) - \psi(z) = 0 \quad (5.33)$$

Theorem 5.2.2 [36] The problem (5.10), (5.32) has a unique solution in $C_A^{2,\alpha}(Q)$ up to an arbitrary additive complex constant, say $C + i\gamma$. This solution is related to the solution $T(z)$ of the 2D problem (5.10), (5.29) by the formulas

$$\varphi(z) \begin{cases} \frac{\lambda_k + 1}{2}(T(z) + iV(z)), & z \in D_k, \quad k = 1, 2, \dots, n \\ T(z) + iV(z), & z \in D \end{cases} \quad (5.34)$$

where $V(z)$ is a harmonic conjugate to $T(z)$. The constant C is the additive arbitrary real constant from the general solution of the 2D problem (5.10), (5.29).

Theorem 5.2.3 [36] General solution of the homogeneous problem (5.21), (5.33) in $C_A^{2,\alpha}(Q)$ has the form

$$\Psi(z) = q_1 \Psi^{(1)}(z) + q_2 \Psi^{(2)}(z) \quad (5.35)$$

where $\Psi^{(1)}(z)$ and $\Psi^{(2)}(z)$ are partial linearly independent solutions of the problem (5.21), (5.33), q_1 and q_2 are arbitrary real constants.

This solution can be fixed by the relation $\Psi^{(j)}(z) = (\varphi^{(j)})'(z)$, where $\varphi^{(j)}(z)$ are as in Theorem 5.2.2; $\varphi^{(1)}(z)$ is a solution of the problem (5.10), (5.32) with $q_1 = 1$, $q_2 = 0$ and $\varphi^{(2)}(z)$ is a solution of the corresponding 2D problem with $q_1 = 0$, $q_2 = 1$.

The decomposition theorem (see representation (5.14)) on the torus generated by the lattice Q was described in Ref. [37]. Any function $T(z)$ which is harmonic in Ω and doubly periodic can be written as

$$T(z) = \operatorname{Re} \left\{ \varphi(z) + \sum_{k=1}^n A_k [\ln \sigma(z - a_k) + a_k \zeta(z - a_k)] \right\}, \quad z \in D \quad (5.36)$$

where σ and ζ are Weierstrass functions (see Section 5.6.1); A_k are real constants satisfying relation (5.15). The function $\varphi(z)$ is analytic in Ω and quasi-periodic. The choice of a branch of the logarithm does not impact on the value $T(z)$ because we actually deal with $\operatorname{Re}\{\ln z\}$ in (5.36). One can choose an arbitrary branch of $\ln(z - a_k)$ and suppose that the cut corresponding to this fixed branch is doubly periodic and has no common points with D_m for each $m \neq k$. Using the representation (5.36), one can reduce periodic boundary value problems for harmonic functions to problems for analytic functions following Section 5.2.4.

5.3

Effective Conductivity Tensor

Although the notation *effective conductivity tensor* is intuitively clear for physicists and engineers, the rigorous mathematical definition of the effective conductivity tensor needs a certain theoretical justification. One of the possible ways for such a justification is the use of homogenization theory. Following Refs. [1,2,17,18,20], consider a periodic composite. Let the linear sizes of the periods be of order ε , where L is the

linear order of the sample D bounded by a simple closed curve Γ . Consider the Dirichlet problem [20, p. 20, Russian edn] in $H_0^1(D)$

$$\nabla(\Lambda_\varepsilon(\mathbf{x})\nabla T_\varepsilon(\mathbf{x})) = 0 \quad (5.37)$$

$$T_\varepsilon(\mathbf{t}) = f(\mathbf{t}), \quad \mathbf{t} \in \Gamma \quad (5.38)$$

Let

$$\Lambda_\varepsilon(\mathbf{x})\nabla T_\varepsilon(\mathbf{x}) \rightharpoonup \hat{\Lambda}\nabla T_0 \text{ in } L_2(D) \quad (5.39)$$

where $\rightharpoonup$ means the weak convergence in $L_2(D)$, $\hat{\Lambda}$ is a constant tensor and T_0 is a solution of the Dirichlet problem

$$\nabla(\hat{\Lambda}\nabla T_0(\mathbf{x})) = 0, \quad T_0(\mathbf{t}) = f(\mathbf{t}), \quad \mathbf{t} \in \Gamma \quad (5.40)$$

Then, the tensor $\hat{\Lambda}$ is called the effective conductivity tensor. The homogenization theory justifies the existence of the weak limit (5.39) and the independence of the limit of the shape of Γ and boundary conditions. For instance, instead of the Dirichlet condition (5.38), the Neumann condition can be taken. Moreover, the homogenization theory implies that $\hat{\Lambda}$ can be calculated by the formula

$$\hat{\Lambda}\mathbf{q} = \langle \Lambda(\mathbf{x})\nabla T(\mathbf{x}) \rangle \quad (5.41)$$

where $\langle F(\mathbf{x}) \rangle$ denote the average over the cell Q

$$\langle F(\mathbf{x}) \rangle = \frac{1}{|Q|} \int_Q F(\mathbf{x}) d\mathbf{x} \quad (5.42)$$

$|Q|$ is the area of Q . The function $T(\mathbf{x})$ is a solution of the quasi-periodic problem (see Section 5.2.5):

$$\begin{aligned} \nabla(\Lambda(\mathbf{x})\nabla T(\mathbf{x})) &= 0, \quad \mathbf{x} \in Q \\ T(x_1 + \alpha, x_2, x_3) - T(x_1, x_2, x_3) &= q_1 \\ T(x_1, x_2 + \beta, x_3) - T(x_1, x_2, x_3) &= q_2 \\ T(x_1, x_2, x_3 + \gamma) - T(x_1, x_2, x_3) &= q_3 \end{aligned} \quad (5.43)$$

Here, $\mathbf{q} = (q_1, q_2, q_3)$ is the external flux. One can see that $\hat{\Lambda}$ is completely determined by (5.41) via solution to three problems (5.43) with $\mathbf{q} = (1, 0, 0)$, $\mathbf{q} = (0, 1, 0)$, $\mathbf{q} = (0, 0, 1)$.

In general, $\hat{\Lambda}$ is a symmetric positively defined tensor. It can be reduced to the diagonal form

$$\hat{\Lambda} = \begin{pmatrix} \hat{\lambda}_1 & 0 & 0 \\ 0 & \hat{\lambda}_2 & 0 \\ 0 & 0 & \hat{\lambda}_3 \end{pmatrix} \quad (5.44)$$

More precisely, there exists a coordinate system in which the tensor $\hat{\Lambda}$ has the diagonal form (5.44). The axes $x'_j (j = 1, 2, 3)$ of this new coordinate system are called *the principal axes*. The component $\hat{\lambda}_j (j = 1, 2, 3)$ is called the conductivity in the x'_j -direction. The tensor ellipsoid, invariants of the tensor and other fundamental properties of tensors can be found in standard courses on tensor algebra (e.g. Ref. [38]).

The tensor $\hat{\Lambda}$ for macroscopically isotropic composites has the form

$$\hat{\Lambda} = \hat{\lambda} \mathbf{I}, \quad (5.45)$$

where $\mathbf{I}$ is the identity tensor, i.e. in this case $\hat{\lambda} = \hat{\lambda}_1 = \hat{\lambda}_2 = \hat{\lambda}_3$. The scalar $\hat{\lambda}$ is called the effective conductivity.

The variational statement of the problem implies the formula

$$\hat{\lambda} \mathbf{q} = \inf_{u \in H^1_{per}(\mathcal{Q})} \langle \lambda(\mathbf{x}) |\nabla u(\mathbf{x})|^2 \rangle = \langle \lambda(\mathbf{x}) |\nabla T(\mathbf{x})|^2 \rangle \quad (5.46)$$

Consider a 2D representative symmetric cell. Then, the periodicity cell problem is reduced to the mixed problem (5.10), (5.30), (5.31) for the domain $\mathcal{Q}$. In this case, the following formula can be used for the effective conductivity in the x_1 -direction:

$$\hat{\lambda}_1 = \frac{4}{\alpha q_1} \int_{-\alpha/4}^{\alpha/4} \lambda \left(x_1, \frac{\beta}{4} \right) \frac{\partial T}{\partial x_1} \left(x_1, \frac{\beta}{4} \right) dx_1 \quad (5.47)$$

This formula expresses that the effective conductivity in the x_1 -direction is equal to the average flux passing along the symmetry segment $x_2 = \frac{\beta}{4}, -\frac{\alpha}{4} < x_1 < \frac{\alpha}{4}$ divided by the jump of the temperature $\frac{q_1}{2}$ per the half-periodicity cell. Similar formulas take place for the conductivities $\hat{\lambda}_2$ and for corresponding coefficients in $\mathbb{R}^3$ (i.e. for 3D composites).

Consider now an application of the formula (5.41) to 2D matrix–inclusion composites. Using the functions $\psi^{(j)}(z)$ described in Theorem 5.2.3, we obtain the components of $\hat{\Lambda}$:

$$\begin{aligned} \hat{\lambda}_{11} - i\hat{\lambda}_{12} &= 1 + 2 \sum_{k=1}^n \rho_k \int_{D_k} \psi^{(1)}(z) dx_1 dx_2, \\ \hat{\lambda}_{22} + i\hat{\lambda}_{21} &= 1 + 2i \sum_{k=1}^n \rho_k \int_{D_k} \psi^{(2)}(z) dx_1 dx_2 \end{aligned} \quad (5.48)$$

For macroscopically isotropic composites, we have

$$\hat{\lambda} = 1 + 2 \sum_{k=1}^n \rho_k \int_{D_k} \psi^{(1)}(z) dx_1 dx_2 \quad (5.49)$$

Consider the case when the inclusions D_k are disks $|z - a_k| < r_k$. Then, application of the mean value theorem to (5.49) yields

$$\hat{\lambda} = 1 + 2 \sum_{k=1}^n \rho_k \pi r_k^2 \psi^{(1)}(a_k) \quad (5.50)$$

Thus one can see that to determine $\hat{\lambda}$ we need only $\psi^{(1)}(a_k)$.

Remark 5.3.1 *The area of the representative cell $|Q|$ does not impact onto the effective conductivity. Hence, it can be normalized to unity.*

5.4

Review of Known Formulas

5.4.1

Laminates

Laminates are described by the local conductivity $\lambda(x_1)$ which depends only on one spatial variable in appropriate coordinates. Let the period of $\lambda(x_1)$ be equal to unity. Then, $\hat{\lambda}$ has the form (5.44) where

$$\hat{\lambda}_1 = \left(\int_0^1 \frac{d\xi}{\lambda(\xi)} \right)^{-1}, \quad \hat{\lambda}_2 = \hat{\lambda}_3 = \int_0^1 \lambda(\xi) d\xi \quad (5.51)$$

Consider the case when $\lambda(x_1)$ takes values λ_1 and λ_2 with the probabilities (concentrations) v_1 and v_2 , respectively. Then, (5.51) becomes

$$\hat{\lambda}_1 = \frac{1}{\frac{v_1}{\lambda_1} + \frac{v_2}{\lambda_2}}, \quad \hat{\lambda}_2 = \hat{\lambda}_3 = v_1 \lambda_1 + v_2 \lambda_2 \quad (5.52)$$

The general theory of laminates is presented in Refs. [2,3,39].

5.4.2

Clausius–Mossotti Approximation (CMA)

We begin with an analytical formula for the effective conductivity of macroscopically isotropic composites known from the eighteenth century. Consider a two-component macroscopically isotropic composite medium consisted of a collection of non overlapping identical balls of conductivity λ_1 imbedded into a host medium of conductivity λ . The effective conductivity $\hat{\lambda}$ of the considered inhomogeneous medium is calculated by the famous Clausius–Mossotti approximation (CMA)

$$\frac{\hat{\lambda}}{\lambda} = \frac{1 + 2\beta v}{1 - \beta v} \quad (5.53)$$

where $\beta = \frac{\lambda_1 - \lambda}{\lambda_1 + 2\lambda}$, v is the concentration of the spheres. This formula is known also as the Maxwell-Garnett or Lorenz-Lorentz formula (for historical remarks see Refs. [40,41]). The formula (5.53) holds for dilute composites when the concentration v is small.

In the 2D case, CMA becomes

$$\frac{\hat{\lambda}}{\lambda} = \frac{1 + \rho v}{1 - \rho v} \quad (5.54)$$

where $\rho = \frac{\lambda_1 - \lambda}{\lambda_1 + \lambda}$ is the 2D contrast parameter (see Eq. (5.22)). Here v is the area concentration of disks on the plane (the section of the fiber composite perpendicular to the direction of fibers).

The Eqs. (5.53) and (5.54) can be deduced in the framework of Maxwell's formalism which is based on solution to the problem for one inclusion. The same method can be applied to inclusions of other shapes.

CMA in 2D Consider a disk of radius r_0 filled in by a material of conductivity λ_1 . The disk $D = \{z \in \mathbb{C} : |z - a| < r_0\}$ is immersed in a material which occupies the domain $D_0 = \{z \in \mathbb{C} : |z - a| > r_0\}$ whose properties are described by the scalar conductivity λ . The whole material is placed into a constant macroscopic flux in the x_1 -direction. Then, the following conjugation conditions hold on the circle $L = \{z \in \mathbb{C} : |z - a| = r_0\}$ orientated in the clockwise sense (see Eq. (5.10)):

$$T^+(t) = T^-(t), \quad \lambda \frac{\partial T^+}{\partial \mathbf{n}}(t) = \lambda_1 \frac{\partial T^-}{\partial \mathbf{n}}(t), \quad t \in L \quad (5.55)$$

We are looking for $T^\pm(z)$ in the following form:

$$T^-(r, \theta) = Ar \cos \theta + B, \quad T^+(r, \theta) = \frac{2\lambda_1}{\lambda_1 + \lambda} \left(r \cos \theta + \frac{C \cos \theta}{r} + E \right) \quad (5.56)$$

where $z = x_1 + ix_2 = a + r(\cos \theta + i \sin \theta)$, and A , B , C and E are undetermined constants. One of the constants B , E can be fixed arbitrarily since the temperature is uniquely determined up to an additive constant. It follows from Eq. (5.56) that the function $T^+(r, \theta)$ has the required behavior at infinity.

$$T^+(r, \theta) \sim \frac{2\lambda_1}{\lambda_1 + \lambda} r \cos \theta = \frac{2\lambda_1}{\lambda_1 + \lambda} x_1, \text{ as } r \rightarrow \infty$$

The conditions (5.55) in polar coordinates become

$$T^+(r_0, \theta) = T^-(r_0, \theta), \quad \lambda \frac{\partial T^+}{\partial r}(r_0, \theta) = \lambda_1 \frac{\partial T^-}{\partial r}(r_0, \theta), \quad 0 \leq \theta < 2\pi \quad (5.57)$$

Substitute Eq. (5.56) in Eq. (5.57) gives

$$\begin{aligned} Ar_0 \cos \theta + B &= \frac{2\lambda_1}{\lambda_1 + \lambda} \left(r_0 \cos \theta + \frac{C \cos \theta}{r_0} + E \right) \\ A \cos \theta &= \frac{2\lambda}{\lambda_1 + \lambda} \left(1 - \frac{C^2}{r_0} \right) \cos \theta, \quad 0 \leq \theta < 2\pi \end{aligned} \quad (5.58)$$

Taking $E = \operatorname{Re} a$, we obtain from Eq. (5.58):

$$A = \frac{4\lambda\lambda_1}{(\lambda_1 + \lambda)^2}, \quad B = \frac{2\lambda_1}{\lambda_1 + \lambda} \operatorname{Re} a, \quad C = \rho r_0^2 \quad (5.59)$$

Therefore, the temperature distribution (5.56) has the form

$$\begin{aligned} T^-(r, \theta) &= \frac{2\lambda_1}{\lambda_1 + \lambda} \left(\frac{2\lambda}{\lambda_1 + \lambda} r \cos \theta + \operatorname{Re} a \right), \quad r \leq r_0 \\ T^+(r, \theta) &= \frac{2\lambda_1}{\lambda_1 + \lambda} \left(r \cos \theta + \frac{\rho r_0^2 \cos \theta}{r} + \operatorname{Re} a \right), \quad r \geq r_0 \end{aligned} \quad (5.60)$$

We introduce the complex potentials:

$$\Phi^-(z) = T^-(z) + iV^-(z), \quad z \in D, \quad \Phi^+(z) = \frac{\lambda_1 + \lambda}{2\lambda_1} (T^+(z) + iV^+(z)), \quad z \in D_0 \quad (5.61)$$

We write Eq. (5.55) in the form of the $\mathbb{R}$ -linear conjugation problem (5.23):

$$\Phi^+(t) = \Phi^-(t) - \rho \overline{\Phi^-(t)}, \quad t \in L \quad (5.62)$$

The function $\Phi^+(z)$ has the principal part $\frac{\lambda_1 + \lambda}{2\lambda_1} z$ at infinity. It is easily checked that the following functions satisfy Eq. (5.62):

$$\Phi^-(z) = (1 - \rho^2)(z - a) + a - \rho \bar{a}, \quad |z - a| \leq r_0, \quad \Phi^+(z) = z + \frac{\rho r_0^2}{z - a}, \quad |z - a| \geq r_0 \quad (5.63)$$

The complex potentials (5.63) correspond to the harmonic functions (5.60) due to Eq. (5.61).

Following Maxwell's approach, we assume that ρr_0^2 is sufficiently small. This is true for dilute media when the inclusions are sparse or for weakly inhomogeneous media when the contrast parameter ρ is small. In the limit case $r_0 = 0$, the function $\Phi^-(z)$ degenerates to a constant and $\Phi^+(z) = z$. In the second limit case $\rho = 0$,

Eq. (5.63) becomes

$$\Phi^-(z) = \Phi^+(z) = z \quad (5.64)$$

The case $r_0 = 0$ can be formally described also by Eq. (5.64). The difference between Eqs. (5.63) and (5.64) for $\Phi^+(z)$ is $\frac{\rho r_0^2}{z-a}$. The real part of the difference in polar coordinates becomes $\rho \frac{r_0^2 \cos \theta}{r}$. Hence, this term can be considered as a perturbation of the complex potential created by the external field due to one inclusion.

Consider the temperature distribution in the medium with n inclusions. The total perturbation term has the form $\rho n \frac{r_0^2 \cos \theta}{r}$ for sufficiently large r far away from all n inclusions. Take now a fictive “homogenized disk” of radius R_0 containing n small inclusions. Repeating the above argument, we will have a perturbation $\hat{\rho} \frac{R_0^2 \cos \theta}{r}$, where $\hat{\rho} = \frac{\hat{\lambda} - \lambda}{\hat{\lambda} + \lambda}$. Supposing that these perturbations are equal, we have

$$\rho n r_0^2 = R_0^2 \hat{\rho} \Leftrightarrow \nu \rho = \frac{\hat{\lambda} - \lambda}{\hat{\lambda} + \lambda} \quad (5.65)$$

where $\nu = n(\frac{R_0}{r_0})^2$ is the area concentration of the disks. Solution to Eq. (5.65) yields CMA (5.54).

CMA in 3D CMA (5.54) can be found in the same way as in the previous part of this subsection. First, we are interested in the solution to the problem for one ball of radius r_0 centered at $\mathbf{x}_0 = (x_1^{(0)}, x_2^{(0)}, x_3^{(0)})$:

$$T^+(\mathbf{t}) = T^-(\mathbf{t}), \quad \lambda \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) = \lambda_1 \frac{\partial T^-}{\partial \mathbf{n}}(\mathbf{t}), \quad |\mathbf{t} - \mathbf{x}_0| = r_0 \quad (5.66)$$

It can be directly checked that its solution has the form

$$T^-(\mathbf{x}) = \frac{3\lambda}{2\lambda + \lambda_1} (x_1 - x_1^{(0)}), \quad T^+(\mathbf{x}) = (x_1 - x_1^{(0)}) \left(1 + \frac{\lambda - \lambda_1}{2\lambda + \lambda_1} \frac{r_0^3}{r^3} \right) \quad (5.67)$$

where $r = |\mathbf{x} - \mathbf{x}_0|$. Here, the external field along the x_1 -axis is also considered.

In the limit cases $r_0 = 0$ and $\lambda_1 = \lambda$, the temperature distribution (5.67) becomes

$$T^+(\mathbf{x}) = T^-(\mathbf{x}) = x_1 - x_1^{(0)} \quad (5.68)$$

Therefore, one can consider the term $\frac{\lambda_1 - \lambda}{2\lambda + \lambda_1} \frac{r_0^3}{r^3}$ as a perturbation due to one ball. Then, the perturbation due to n balls $n\beta \frac{r_0^3}{r^3}$ can be equal to the perturbation of the

homogenized ball:

$$\beta n r_0^3 = R_0^3 \frac{\hat{\lambda} - \lambda}{\hat{\lambda} + 2\lambda} \Leftrightarrow \nu \beta = \frac{\hat{\lambda} - \lambda}{\hat{\lambda} + 2\lambda} \quad (5.69)$$

where $\nu = n(\frac{r_0}{R_0})^3$ is the volume concentration of the balls. Solution to equation (5.69) yields CMA (5.53).

Remark 5.4.1 *Application of Maxwell's approach to composite media with elliptic inclusions is given in Ref. [42]. One can find there approximate analytical formulas for the effective conductivity. Other shapes of inclusions are studied in Ref. [43] in terms of Pólya–Szegő's matrix. This matrix expresses the effective conductivity tensor for dilute inclusions and corresponds to CMA.*

5.4.3

Effective Medium Theory (EMT)

The effective medium theory (EMT) is based on local study of the composites and porous media when an inclusion is embedded in a homogeneous medium whose effective conductivity is unknown and to be determined by averaging the local structure. Application of EMT leads to analytical formulas for the effective conductivity. It was originated by Bruggeman [44] and developed by Kirkpatrick [45] who proposed approximating the medium by square or cubic network (see Section 5). Self-consistent methods, the method of Mori–Tanaka [46], differential effective medium methods and their relations and extensions were discussed in Ref. [47]. We discuss here the cases of circular and spherical inclusions separately.

EMT in 2D Consider a 2D basic element in the complex plane $\mathbb{C}$ in the form of a disk of radius r_k filled in by a material of conductivity λ_k , i.e. the number k is fixed. The disk $D_k = \{z \in \mathbb{C} : |z - a_k| < r_k\}$ is immersed in a material which occupies the domain $\Omega_k = \{z \in \mathbb{C} : |z - a_k| > r_k\}$ whose properties are described by the scalar conductivity $\hat{\lambda}$ (the effective conductivity to be determined later). The whole material is placed into a constant macroscopic flux in the x_1 -direction. Then, the following conjugation conditions hold on the fixed circle $L_k = \{z \in \mathbb{C} : |z - a_k| = r_k\}$ orientated in the clockwise sense (compare with Eq. (5.55)):

$$T^+(t) = T^-(t), \quad \hat{\lambda} \frac{\partial T^+}{\partial \mathbf{n}}(t) = \lambda_k \frac{\partial T^-}{\partial \mathbf{n}}(t), \quad t \in L_k \quad (5.70)$$

The problem (5.70) has been solved in Section 5.4.2 (see Eq. (5.60)). In polar coordinates $z = x_1 + ix_2 = a_k + r(\cos \theta + i \sin \theta)$, its solution has the form

$$\begin{aligned} T^-(r, \theta) &= \frac{2\lambda_k}{\lambda_k + \hat{\lambda}} \left(\frac{2\hat{\lambda}}{\lambda_k + \hat{\lambda}} r \cos \theta + \operatorname{Re} a_k \right) \\ T^+(r, \theta) &= \frac{2\lambda_k}{\lambda_k + \hat{\lambda}} \left(r \cos \theta + \frac{\Delta_k r_k^2 \cos \theta}{t} + \operatorname{Re} a_k \right) \end{aligned} \quad (5.71)$$

where $\Delta_k = \frac{\hat{\lambda} \lambda_k}{\hat{\lambda} + \lambda_k}$.

The problem (5.70) in terms of the complex potentials

$$\Phi^-(z) = T^-(z) + iV^-(z)z \in D_k, \quad \Phi^+(z) = \frac{\lambda_k + \hat{\lambda}}{2\lambda_k} (T^+(z) + iV^+(z)), \quad z \in \Omega_k \quad (5.72)$$

becomes

$$\Phi^+(t) = \Phi^-(t) - \Delta_k \overline{\Phi^-(t)}, \quad t \in L_k \quad (5.73)$$

It follows from Eq. 5.63 that

$$\Phi^-(z) = (1 - \Delta_k^2)(z - a_k) + a_k - \Delta_k \overline{a_k}, \quad \Phi^+(z) = z + \frac{\Delta_k r_k^2}{z - a_k} \quad (5.74)$$

The residue of $\Phi^+(z)$ at $z = a_k$ is equal to $\Delta_k r_k^2$. It expresses the dipole moment of the complex potential $\Phi^+(z)$. Up to now it was assumed that the number k is fixed. Let us consider infinitely many disks packing the plane, i.e. each point of the plane belongs to one disk. Let all disks be divided into n types characterized by the radius r_k , and having conductivity λ_k . Let v_k denote the concentration of the disks of the k -th type uniformly distributed on the plane. One can consider v_k as the area probability of the k -th type. Then, $\sum_{k=1}^n v_k = 1$. We are interested in the total dipole moment corresponding to disks. The dipole moment of each disk is approximated by $\Delta_k r_k^2$ and the dipole moment of the “level” (phase) k is proportional to $\Delta_k v_k$. Supposing that the total moment created by each level vanishes, we have

$$\sum_{k=1}^n v_k \Delta_k = 0 \Leftrightarrow \sum_{k=1}^n v_k \frac{\hat{\lambda} - \lambda_k}{\hat{\lambda} + \lambda_k} = 0 \quad (5.75)$$

The effective conductivity $\hat{\lambda}$ is the solution of Eq. (5.75).

The relation (5.75) admits the following continuous interpretation:

$$\int_0^\infty v(\lambda) \frac{\hat{\lambda} - \lambda}{\hat{\lambda} + \lambda} d\lambda = 0 \quad (5.76)$$

where $v(\lambda)$ is the density function of the random variable λ .

Example 5.4.2 Consider a two-phase material each phase of which takes the same area. Then, $n=2$, $v_1 = v_2 = \frac{1}{2}$ and Eq. (5.75) yields the geometric mean for the effective conductivity

$$\hat{\lambda} = \sqrt{\lambda_1 \lambda_2} \quad (5.77)$$

Example 5.4.3 Following Ref. [47], consider the lognormal distribution of local conductivity

$$v(\lambda) = \frac{1}{b\lambda\sqrt{\pi}} \exp\left(-\frac{(\ln\lambda - a)^2}{2b^2}\right) \quad (5.78)$$

with positive parameters a and b . We now prove that Eq. (5.76) with $v(\lambda)$ given by Eq. (5.78) has the unique solution

$$\hat{\lambda} = \exp a \quad (5.79)$$

The existence and uniqueness for Eq. (5.76) follows from physical observation that the effective conductivity exists for macroscopically isotropic media. Let us change the variable in the integral (5.76) $\lambda = \frac{\exp 2a}{t}$ and use the relation $v(t) = \frac{\exp 2a}{t^2} v\left(\frac{\exp 2a}{t}\right)$ for the function (5.78). Then Eq. (5.76) becomes

$$\int_0^\infty v(t) \frac{t - \frac{\exp 2a}{\hat{\lambda}}}{t + \frac{\exp 2a}{\hat{\lambda}}} dt = 0 \quad (5.80)$$

Since Eqs. (5.76) and (5.80) have a unique solution, these equations give the same result $\hat{\lambda} = \frac{\exp 2a}{\lambda}$ which implies Eq. (5.79). It follows from Section 5.4.4 that the formula (5.80) is exact for the lognormal distribution.

EMT in 3D Following the previous part of this subsection and Ref. [6], we construct an effective medium approximation in 3D case. It can be directly checked that the solution of the problem

$$T^+(\mathbf{t}) = T^-(\mathbf{t}), \quad \hat{\lambda} \frac{\partial T^+}{\partial \mathbf{n}}(\mathbf{t}) = \lambda_k \frac{\partial T^-}{\partial \mathbf{n}}(\mathbf{t}), \quad \mathbf{t} \in L_k \quad (5.81)$$

for the sphere L_k of radius r_k centered at $\mathbf{x}_k = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)})$ has the form

$$T^-(\mathbf{x}) = \frac{3\hat{\lambda}}{2\hat{\lambda} + \lambda_k} (x_1 - x_1^{(k)}), \quad T^+(\mathbf{x}) = (x_1 - x_1^{(k)}) \left(1 + \frac{\hat{\lambda} - \lambda_k}{2\hat{\lambda} + \lambda_k} \frac{r_k^3}{r^3}\right) \quad (5.82)$$

where $r = |\mathbf{x} - \mathbf{x}_k|$. Here, for simplicity, the external field is taken along the x_1 -axis.

The dipole moment corresponding to the phase of conductivity λ_k is proportional to $v_k \frac{\hat{\lambda} - \lambda_k}{2\hat{\lambda} + \lambda_k}$. Equating the total moment to zero, we obtain an equation for the effective conductivity $\hat{\lambda}$:

$$\sum_{k=1}^n v_k \frac{\hat{\lambda} - \lambda_k}{2\hat{\lambda} + \lambda_k} = 0 \quad (5.83)$$

The latter formula can be extended to the continuous phase case

$$\int_0^\infty v(\lambda) \frac{\hat{\lambda} - \lambda}{2\hat{\lambda} + \lambda} d\lambda = 0 \quad (5.84)$$

Remark 5.4.4 *The differential method is closely related to EMT. One can find analytical formulas for different types of composite media and references for instance in Refs. [41,42].*

5.4.4

Duality Theory for 2D Media

Keller–Mathéron Theory The theory of duality transformation of 2D media was discovered by Keller [48] for two-phase media and independently by Mathéron [49] for general media. It is based on the observation that a divergent free field produces a curl-free field when it is rotated locally by 90° . Application of this theory yields an expression for the effective conductivity of a two-phase medium when phases are interchanged. The famous square-root formula (5.77) was deduced by Dykhne [50] by use of duality. It is exact for the square checkerboard.

Following Mathéron [49], we introduce the resistivity tensor $H(\mathbf{x}) = \Lambda^{-1}(\mathbf{x})$ and treat the local tensors as random functions of $\mathbf{x}$. Consider a 2D medium when the following hypothesis is fulfilled:

(H₁) *The random fields $\Lambda(\mathbf{x})\langle\Lambda(\mathbf{x})\rangle^{-1}$ and $H(\mathbf{x})\langle H(\mathbf{x})\rangle^{-1}$ have the same spatial distribution.*

Then [20,47,51,52],

$$|\hat{\Lambda}| = \frac{|\langle\Lambda(\mathbf{x})\rangle|}{|\langle\Lambda(\mathbf{x})|\Lambda(\mathbf{x})|^{-1}\rangle|} \quad (5.85)$$

where $|\cdot|$ denotes the determinant of the matrix, $\langle\cdot\rangle$ is the spatial average (5.42). In the particular case where $\Lambda(\mathbf{x})$ takes only two constant values $\lambda_1\mathbf{I}$ and $\lambda_2\mathbf{I}$ with the same probability $\frac{1}{2}$ we obtain Keller's identity [48]

$$\hat{\lambda}_1\hat{\lambda}_2 = \lambda_1\lambda_2 \quad (5.86)$$

Here, $\hat{\lambda}_1$ is the effective conductivity of the medium in the x_1 -direction, $\hat{\lambda}_2$ is the effective conductivity in the x_2 -direction of another medium which is produced from the original one by exchanging the phases with different conductivities λ_1 and λ_2 .

Consider a medium for which the hypothesis (H₁) and also the following hypothesis are valid:

(H₂) *The random fields $\Lambda(\mathbf{x})$ is invariant under rotations.*

Then, the effective tensor is isotropic and [49]

$$\hat{\lambda} = \sqrt{\lambda_0 h_0} \quad (5.87)$$

where the scalars λ_0 and h_0 denote the average conductivity and resistance over the representative cell, namely $\langle \Lambda(\mathbf{x}) \rangle = \lambda_0 \mathbf{I}$, $\langle H(\mathbf{x}) \rangle = h_0 \mathbf{I}$. In the particular case where $\Lambda(\mathbf{x})$ takes only two constant values $\lambda_1 \mathbf{I}$ and $\lambda_2 \mathbf{I}$ with the same probability $\frac{1}{2}$, Eq. (5.87) yields Eq. (5.77).

The following duality transformation between two different conductivity problems was proposed by Milton [3]. Let $\Lambda(\mathbf{x})$ be the conductivity tensor in a medium; define the conductivity tensor $\Lambda'(\mathbf{x})$ by

$$\Lambda'(\mathbf{x}) = [a\Lambda(\mathbf{x}) + b\mathbf{R}][c\mathbf{I} + d\mathbf{R}\Lambda(\mathbf{x})]^{-1} \quad (5.88)$$

where a, b, c, d are constants and $\mathbf{R}$ is the matrix for 90° rotation. Milton proved that their effective conductivity tensors are also related by Eq. (5.88).

The effective conductivity of the three-phase tessellation is conjectured to be an algebraic function in Ref. [53]. Other relations of the theory of duality transformations and their applications are discussed in Refs. [47,54–57] and works cited therein.

Craster–Obnosov Formulas It was noted in 1996 [58,59] that the study of the few-phases checkerboard composites can be reduced to the matrix Riemann–Hilbert problem of analytic function theory. Craster and Obnosov in a series the papers [59–65] deduced exact formulas for the effective conductivity tensor based on the explicit representations of the local fields for various types of such composites.

Consider a doubly periodic four-phase checkerboard composite when the representative rectangle has the lengths of the sides α, α^{-1} (see Figure 5.1).

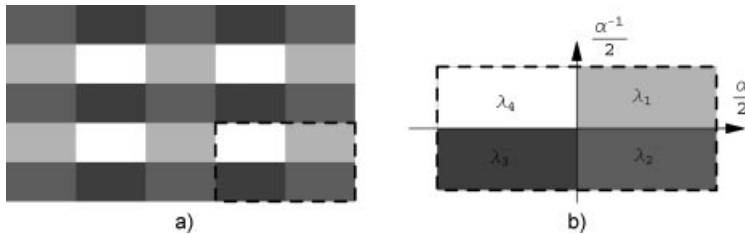


Figure 5.1 Checkerboard four-phase medium: (a) doubly checkerboard; (b) representative cell.

Let the local conductivity $\lambda = \lambda(\mathbf{x})$ take the value λ_j in the j -phase ($j = 1, 2, 3, 4$). Following Ref. [59], we use the complete elliptic integral:

$$K(m) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-m^2\sin^2\theta}}$$

where the parameter m is implicitly defined via the equation $K(m)/K(1-m) = \alpha^2$. We introduce also the parameters

$$\begin{aligned}\sigma_1 &= \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4, & \sigma_2 &= \lambda_1\lambda_3 + \lambda_2\lambda_4, \\ \sigma_3 &= \lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4\end{aligned}\quad (5.89)$$

The parameter ϑ is introduced implicitly via $\cos\pi\vartheta = 1 - 2\sigma_2^2(\sigma_1\sigma_3 + \sigma_2^2)^{-1}$. We introduce the function

$$k(m, \vartheta) = \frac{P_{\frac{\vartheta}{2}-\frac{1}{2}}(2m-1)}{P_{\frac{\vartheta}{2}-\frac{1}{2}}(1-2m)} \quad (5.90)$$

where P_μ is the Legendre function of the first kind. The effective conductivity is explicitly given by the formulas

$$\hat{\lambda}_1 = \frac{1}{\alpha^2 k(m, \vartheta)} \left[\frac{(\lambda_1 + \lambda_2)(\lambda_3 + \lambda_4)}{(\lambda_2 + \lambda_3)(\lambda_4 + \lambda_1)} \right]^{\frac{1}{2}} \left(\frac{\sigma_1}{\sigma_3} \right)^{\frac{1}{2}} \quad (5.91)$$

$$\hat{\lambda}_2 = \alpha^2 k(m, \vartheta) \left[\frac{(\lambda_2 + \lambda_3)(\lambda_4 + \lambda_1)}{(\lambda_1 + \lambda_2)(\lambda_3 + \lambda_4)} \right]^{\frac{1}{2}} \left(\frac{\sigma_1}{\sigma_3} \right)^{\frac{1}{2}} \quad (5.92)$$

It is worth noting that for the square checkerboards $\alpha = 1$ implies $m = \frac{1}{2}$. Hence, $k(\frac{1}{2}, \vartheta) = 1$ and Eqs. (5.91) and (5.92) become simple algebraic functions of λ_j .

Other special cases such as $\lambda_2 = \lambda_4$, highly contrasting phases and other new formulas are discussed in the papers cited above. In particular, nonconducting or perfectly conducting strips between phases in four-phase checkerboards [61], triangle structures [62,64] have been explicitly studied. The case $\lambda_2 = \lambda_3 = \lambda_4$ corresponds to composites with rectangular inclusions of the concentration $\frac{1}{4}$. The effective properties of medium with quadratic holes with arbitrary concentration were explicitly calculated in Ref. [66] by application of conformal mappings.

5.5

Network Approximations

Network approximations for evaluation of the temperature field in composites and porous media is based on the replacement of the 3D solid material by Kirchhoff's

discrete circuit presented by a graph. Such approximations can be applied for instance to two-phase composites with high contrast parameter when the conductivity of inclusions is much greater than the conductivity of matrix and the inclusions generate clusters, i.e. the inclusions are closed, and the heat is transferred mainly along paths connecting them. The vertices of the graph correspond to the inclusions and the paths correspond to one-dimensional edges of the graph.

Various authors [67–71] developed continuum percolation models taking into account the spatial geometry of media. The saddle points of the smooth phase function were used in Ref. [67] as elementary blocks of the network. By contrast, the capacity of the pair of inclusions were used in Refs. [68–71] as the conductivity of the basic paths conducting the heat.

Following Ref. [69], we discuss macroscopically isotropic 2D composites with random nonoverlapping identical circular inclusions of radii r . The temperature field between the neighboring disks D_i and D_j is described by Keller's formula [72] for the specific flux:

$$g_{ij} = \pi \sqrt{\frac{r}{\delta_{ij}}} \quad (5.93)$$

where δ_{ij} is the distance between the disks.

The definition of neighbor disks is introduced via 2D Voronoi tessellation. It is illustrated by Figure 5.2, where the centers of the disks are considered as vertices of the graph Γ . The domain Q is divided into polygonal regions. Each of the polygonal regions contains only one vertex and points which are closer to this vertex than to one another. Hence, each edge of the graph Γ is divided by a side of the polygons by two equal segments. Moreover, the edge and the side are perpendicular and all points of the side are equidistant from the corresponding vertices. The graph Γ' consisting of the sides of the polygons is called the dual graph to the graph Γ .

Let i be the number of the disk D_i in the representative cell Q ($i = 1, 2, \dots, N$). Divide the set $\{i = 1, 2, \dots, N\}$ onto the subsets I , S^+ and S^- , where $S^\pm$ corresponds to the

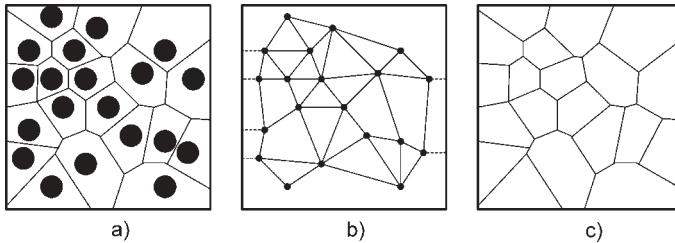


Figure 5.2 Continuous percolation model: (a) nonoverlapping disks and Voronoi tessellation; (b) Delaunay graph Γ , its vertices are centers of the disks; (c) dual graph Γ' whose edges coincide with the sides of Voronoi's polygons.

disks which are closed to the boundary edges $x = \pm \frac{1}{2}$ of the cell Q and I corresponds to internal disks. The discrete temperature distribution $T(\mathbf{x}) = t_i$, $\mathbf{x} \in D_i$, satisfies the system of linear algebraic equations:

$$\sum_{j \in A(i)} g_{ij}(t_i - t_j) = 0, \quad \text{for } i \in I, \quad t_i = \pm \frac{1}{2}, \quad \text{for } i \in S^{\pm} \quad (5.94)$$

where g_{ij} has the form (5.93), $A(i)$ denotes the set of vertices which are adjacent to the vertex i , i.e. other vertices of the edges containing the vertex i . The first Eq. (5.94) correspond to the flux in the necks between inclusions, the second to the boundary conditions. Actually, Berlyand and co-workers, [68–71] used a more complicated model taking into account interaction with the boundary of Q .

The effective conductivity is given by the following asymptotic formula:

$$\hat{\lambda} = \frac{1}{4} \sum_{i,j} g_{ij}(t_i - t_j)^2 + O(1) + O\left(\sqrt{\frac{\delta}{r}}\right), \quad \text{as } \delta \rightarrow 0 \quad (5.95)$$

where $\delta = \max(\delta_{ij})$. Each term $\frac{1}{4}g_{ij}(t_i - t_j)^2$ is of order $O\left(\sqrt{\frac{r}{\delta}}\right)$. It comes from the formula for the energy of a condenser $E = \frac{1}{2}CV^2$, where C is its capacity, V is the difference of potentials. The additional multiplier $\frac{1}{2}$ is put in Eq. (5.95), since each term is taken two times.

The formula (5.95) can be used for composites with a high concentration of inclusions and a high contrast parameter. First, one has to solve the system (5.94) with respect to t_i where the coefficients g_{ij} are determined by the distances between inclusions δ_{ij} , i.e. the geometry of the medium. Then, t_i are substituted into Eq. (5.95).

The correspondence of the discrete model to the original continuum medium with circular inclusions had been rigorously justified in Refs. [68–71]. Other shapes of inclusions and 3D composites were also discussed by a similar method. It follows from formula (5.93) that the capacity tends to infinity as δ_{ij} tends to zero. This means that the heat is mainly transferred through the necks between inclusions. However, the relationship between the discrete and continuous models is not direct for general problems. Kolpakov [73] investigated this problem by estimation of the capacity of the pairs of inclusions when the distance between the inclusions δ_{ij} tends to zero. He showed that the capacity tends to zero if $\delta_{ij} \rightarrow 0$ in 2D. However, this correspondence fails for the pair cone-half space in 3D.

In porous media, instead of the perfectly conducting inclusions, isolating holes are considered. Then, the conducting solid phase can be approximated by the graph Γ' . Pores can be filled by heated gases. Then, other types of problems can arise. It is worth noting that the latter problems are not studied as deeply as problems for porous media with perfectly conducting inclusions discussed above.

5.6

Doubly Periodic Problems

5.6.1

Introduction to Elliptic Function Theory

Elliptic functions [74,75] are doubly periodic meromorphic functions with the periods ω_1, ω_2 whose ratio ω_2/ω_1 is not a real number (it should be mentioned that Jacobi's theorem says that there is no single-valued analytic function with more than two periods).

Let us recall now some general properties of doubly periodic functions. Let $f(z)$ be a single-valued analytic function with two periods ω_1/ω_2 , $\text{Im } \omega_2/\omega_1 > 0$. Then

$$f(z+w) = f(z), \quad \forall w = m_1\omega_1 + m_2\omega_2, \quad m_1, m_2 \in \mathbb{Z}$$

Any parallelogram with points $z_0, z_0 + \omega_1, z_0 + \omega_1 + \omega_2, z_0 + \omega_2$ as its vertices is called a *parallelogram of periods* (and also a *fundamental cell*, whenever $z_0 = 0$).

Weierstrass $\wp$ -function The Weierstrass $\wp$ -function can be represented in the form of a series:

$$\wp(z) = \frac{1}{z^2} + \sum'_{m_1, m_2} \left[\frac{1}{(z - m_1\omega_1 - m_2\omega_2)^2} - \frac{1}{(m_1\omega_1 + m_2\omega_2)^2} \right] \quad (5.96)$$

where $\sum'_{m_1, m_2}$ means that summation is performed over all integers $m_1, m_2 \in \mathbb{Z}$ except $m_1, m_2 = 0$. The properties (a) to (e) follow directly from Eq. (5.96):

- $\wp(z)$ is a doubly periodic function with the only pole $m_1\omega_1 + m_2\omega_2$.
- $\wp(z)$ is an even function of order 2.
- Its derivative $\wp'$ is an odd function of order 3.
- In the neighborhood of the origin its principal part is equal to $\frac{1}{z^2}$.
- $\wp(z) - \frac{1}{z^2}$ tends to zero as $z \rightarrow 0$.
- It is an inverse function to the elliptic integral:

$$z = \int_{\infty}^{\zeta} \frac{dx}{\sqrt{4x^3 - g_2x - g_3}} \quad (\zeta = \wp(z)) \quad (5.97)$$

where

$$g_2 = 60 \sum'_{m_1, m_2} \frac{1}{(m_1\omega_1 + m_2\omega_2)^4}, \quad g_3 = 140 \sum'_{m_1, m_2} \frac{1}{(m_1\omega_1 + m_2\omega_2)^6} \quad (5.98)$$

The functions $\wp(z)$ and $\wp'$ are related by the following algebraic relation:

$$\wp'^2(z) = 4\wp^3(z) - g_2\wp(z) - g_3 \quad (5.99)$$

Weierstrass ζ -function The Weierstrass ζ -function (which should not be confused with the well-known Riemann ζ -function playing an important role in the description of prime numbers) is defined by integration of the Weierstrass $\wp$ -function, namely

$$\zeta(z) = \frac{1}{z} - \int_0^z \left\{ \wp(z) - \frac{1}{z^2} \right\} dz \quad (5.100)$$

Differentiating Eq. (5.100), we have $\zeta'(z) = -\wp(z)$. Therefore, the Weierstrass ζ -function is an odd function ($\zeta(-z) = -\zeta(z)$) having only the one pole in the parallelogram of periods (of the $\wp$ -function (!)) with residue 1. Hence, the ζ -function cannot be elliptic; sometimes it is called *quasi-periodic* since the following relations are valid:

$$\zeta(z + \omega_1) = \zeta(z) + 2\eta_1, \quad \zeta(z + \omega_2) = \zeta(z) + 2\eta_2 \quad (5.101)$$

where the constants η_1, η_2 are equal $\eta_1 = \zeta(\omega_1/2), \eta_2 = \zeta(\omega_2/2)$.

Weierstrass σ -function This function of the Weierstrass collection is obtained due to line integration of $\zeta(z) - \frac{1}{z}$ along an arbitrary curve starting from the origin and not passing through any pole of the integrand. To avoid multi-valuedness, $\sigma(z)$ is defined as follows:

$$\log \frac{\sigma(z)}{z} = \int_0^z \left\{ \zeta(z) - \frac{1}{z} \right\} dz \quad (5.102)$$

Differentiation formula has in this case the form $\frac{\sigma'(z)}{\sigma(z)} = \zeta(z)$. The σ -function is an odd function having no singularity in any bounded domain and only zeroes at $z = m_1\omega_1 + m_2\omega_2$. Thus, it is also not an elliptic function. The following holds with the same constants as for ζ -function: $\sigma(z + \omega_1) = -e^{2\eta_1(z + \omega_1)}\sigma(z), \sigma(z + \omega_2) = -e^{2\eta_2(z + \omega_2)}\sigma(z)$.

θ -function In practice, it is often supposed that one of the periods of an elliptic function is real. It can be realized by performing the following changes of variables: $v = \frac{z}{\omega_1}, \quad \tau = \frac{\omega_2}{\omega_1}$. Then, in the variable v , the elliptic function will have the periods 1 and τ , still supposing that $\text{Im } \tau > 0$. In this variable, the θ -function is defined in form of a series:

$$\theta(v) = i \sum_{n=-\infty}^{\infty} (-1)^n q^{\left(n-\frac{1}{2}\right)^2} e^{(2n-1)\pi v i} \quad (5.103)$$

where $q = e^{\pi i \tau}$. There is a connection between the θ -function and σ -function given by the formula:

$$\sigma(z) = \frac{\omega_1}{\theta'(0)} e^{\frac{\pi z^2}{\omega_1}} \theta\left(\frac{z}{\omega_1}\right) \quad (5.104)$$

Hence, the θ -function has no poles at any bounded domain (and is not an elliptic function). From the definition (5.103) of the θ -function, it follows that $\theta(v+1) = -\theta(v)$, $\theta(v+\tau) = -\frac{1}{q} e^{-2\pi v i} \theta(v)$. The points $v = m_1 + m_2 \tau$ are the only zeros of the θ -function.

Classical Eisenstein–Rayleigh Sums It is convenient to use the elliptic functions in the form of the *Eisenstein series* introduced by Eisenstein in 1847 and developed by Weil [76]. The classical lattice sums (the Eisenstein sums) were applied to calculation of the effective conductivity tensor by Rayleigh [77] (see also Refs. [78,79,95,96]) when a representative cell contains one inclusion.

In the present subsection, we introduce the fundamental parameters of the elliptic function theory following Weil [76] and Akhiezer [74]. Consider a lattice $\mathcal{Q}$ which is defined by two fundamental translation vectors expressed by complex numbers ω_1 and ω_2 on the complex plane $\mathbb{C}$. For definiteness, we assume that $\text{Im} \tau > 0$, where $\tau = \omega_2/\omega_1$. We introduce the $(0,0)$ cell $Q_{(0,0)} = \{z = t_1 \omega_1 + t_2 \omega_2; -1/2 < t_j < 1/2 (j=1,2)\}$. The lattice $\mathcal{Q}$ consists of the cells $Q_{(m_1, m_2)} = \{z \in \mathbb{C} : z - m_1 \omega_1 - m_2 \omega_2 \in Q_{(0,0)}\}$, where m_1 and m_2 run over integer numbers.

The Eisenstein summation method is defined as follows:

$$\sum_{m_1, m_2} = \lim_{N \rightarrow \infty} \sum_{m_2 = -N}^N \left(\lim_{M \rightarrow \infty} \sum_{m_1 = -M}^M \right) \quad (5.105)$$

Using this summation, we introduce

$$S_n(\omega_1, \omega_2) = \sum'_{m_1, m_2} (m_1 \omega_1 + m_2 \omega_2)^{-n} \quad (5.106)$$

where m_1 and m_2 run over all integer numbers except the pair $m_1 = m_2 = 0$, $n = 2, 3, \dots$. The sum (5.106) with $n = 2$ is conditionally hence slowly convergent. The formula deduced in Ref. [80] $S_2(\omega_1, \omega_2) = \frac{2}{\omega_1} \zeta\left(\frac{\omega_1}{2}\right)$ is efficient in computations. Rylko [81] deduced another efficient formula:

$$S_2(\omega_1, \omega_2) = \left(\frac{\pi}{\omega_1}\right)^2 \left(\frac{1}{3} - 8 \sum_{m=1}^{\infty} \frac{m q^{2m}}{1 - q^{2m}}\right), \text{ where } q = \exp(\pi i \tau) \quad (5.107)$$

The sums (5.106) with $n > 2$ are absolutely convergent. It is known that $S_n(\omega_1, \omega_2) = 0$ for odd n . For even n , the Eisenstein–Rayleigh sums (5.106) can be easily calculated

through the rapidly convergent infinite sums (see Eq. (5.98))

$$g_2 = g_2(\omega_1, \omega_2) = \left(\frac{\pi}{\omega_1}\right)^4 \left(\frac{4}{3} + 320 \sum_{m=1}^{\infty} \frac{m^3 q^{2m}}{1 - q^{2m}}\right) \quad (5.108)$$

$$g_3 = g_3(\omega_1, \omega_2) = \left(\frac{\pi}{\omega_1}\right)^6 \left(\frac{8}{27} - \frac{448}{3} \sum_{m=1}^{\infty} \frac{m^5 q^{2m}}{1 - q^{2m}}\right) \quad (5.109)$$

Then, $S_4(\omega_1, \omega_2) = \frac{1}{60} g_2(\omega_1, \omega_2)$, $S_6(\omega_1, \omega_2) = \frac{1}{1400} g_3(\omega_1, \omega_2)$. The sums $S_{2n}(\omega_1, \omega_2)$ ($n \geq 4$) are calculated by the recurrence formula:

$$S_{2n}(\omega_1, \omega_2) = \frac{3}{(2n+1)(2n-1)(n-3)} \sum_{m=2}^{n-2} (2m-1)(2n-2m-1) S_{2m} S_{2(n-m)} \quad (5.110)$$

Remark 5.6.1 The series (5.106) with $n = 2$ is conditionally convergent [82]. The possibility of its calculation by using (5.107) is justified in. A formula for nonperiodic (random) arrays to properly define S_2 is discussed in Ref. [83].

Weierstrass functions can be expressed as Taylor expansions:

$$\begin{aligned} \ln \sigma(z) &= \ln z - \sum_{n=2}^{\infty} \frac{S_{2n}}{2n} z^{2n}, \quad \zeta(z) = \frac{1}{z} - \sum_{n=2}^{\infty} S_{2n} z^{2n-1}, \\ \wp(z) &= \frac{1}{z^2} + \sum_{n=2}^{\infty} (2n-1) S_{2n} z^{2n-2} \end{aligned} \quad (5.111)$$

The formulas (5.111) are not used for calculating the Weierstrass functions. For instance, $\sigma(z)$ is better computed by (5.104), because the θ -function can be computed by a very fast formula (5.103).

Eisenstein Series In the following, we summarize the main facts of the Eisenstein series theory following Weil [76]. The Eisenstein series are defined as follows:

$$E_n(z; \omega_1, \omega_2) = \sum_{m_1, m_2} (z - m_1 \omega_1 - m_2 \omega_2)^{-n}, \quad n = 2, 3, \dots \quad (5.112)$$

The Eisenstein summation method (5.105) is applied to $E_2(z; \omega_1, \omega_2)$. The series $E_n(z; \omega_1, \omega_2)$ for $n = 3, 4, \dots$ as a function in z converge absolutely and almost uniformly in the domain $\mathbb{C} \setminus \cup_{m_1, m_2} (m_1 \omega_1 + m_2 \omega_2)$. Each of the functions (5.112) is doubly periodic and has a pole of order n at $z = 0$. However, further it will be convenient to define the value of $E_n(z; \omega_1, \omega_2)$ at the point zero as follows:

$$E_n(0; \omega_1, \omega_2) = S_n(\omega_1, \omega_2) \quad (5.113)$$

The Eisenstein functions of the even order $E_{2n}(z)$ can be presented in the form of the series:

$$E_{2n}(z) = \frac{1}{z^{2n}} + \sum_{k=0}^{\infty} \sigma_k^{(n)} z^{2(k-1)} \quad (5.114)$$

where

$$\sigma_k^{(n)} = \frac{(2n+2k-3)!}{(2n-1)!(2k-2)!} S_{2(n+k-1)} \quad (5.115)$$

The Eisenstein series and the Weierstrass function $\wp(z; \omega_1, \omega_2)$ are related by the identities

$$\begin{aligned} E_2(z; \omega_1, \omega_2) &= \wp(z; \omega_1, \omega_2) + S_2(\omega_1, \omega_2), \\ E_n(z; \omega_1, \omega_2) &= \frac{(-1)^n}{(n-1)!} \frac{d^{n-2}}{dz^{n-2}} \wp(z; \omega_1, \omega_2) \end{aligned} \quad (5.116)$$

Generalized Eisenstein–Rayleigh Sums We now proceed to introduce one of the most important mathematical objects of the present section, the generalized Eisenstein–Rayleigh sums. Consider a set of points a_k ($k = 1, 2, \dots, N$) in the cell Q . Let p be a natural number; k_s runs over 1 to N , $n_j = 2, 3, \dots$. Let $\mathbf{C}$ be the operator of complex conjugation. The value

$$e_{m_1 \dots m_q} := N^{-[1 + \frac{1}{2}(m_1 + \dots + m_q)]} \sum_{k_0 k_1 \dots k_q} E_{m_1}(a_{k_0} - a_{k_1}) \overline{E_{m_2}(a_{k_1} - a_{k_2})} \dots \mathbf{C}^q E_{m_q}(a_{k_{q-1}} - a_{k_q}) \quad (5.117)$$

is called the generalized Eisenstein–Rayleigh sum. The parameters ω_1 and ω_2 are omitted in E_n . According to (5.113), $e_n(\omega_1, \omega_2)$ becomes the classical Eisenstein–Rayleigh sum $S_n(\omega_1, \omega_2)$ in the case $N=1$.

We are also interested in the normalized Eisenstein series (compare to Eq. (5.103):

$$E_n(z; 1, \tau) = \sum_{m_1, m_2} (z - m_1 - m_2 \tau)^{-n}, \quad n = 2, 3, \dots \quad (5.118)$$

We have the relations

$$E_n(z; \omega_1, \omega_2) = \omega_1^{-n} E_n\left(\frac{z}{\omega_1}; 1, \tau\right), \quad e_{n_1 \dots n_p}(\omega_1, \omega_2) = \omega_1^{-2k} e_{n_1 \dots n_p}(1, \tau) \quad (5.119)$$

where $2k := n_1 + \dots + n_p$. Note that we shall need further only the even sums $n_1 + \dots + n_p$.

Remark 5.6.2 *Berdichevskij [84] constructed three-dimensional counterparts of the elliptic functions which could be used for three-dimensional conductivity and elasticity problems. Huang [85] proposed exact integral formulas for three-dimensional lattice sums. His examples show that simple quadrature rules with modest numbers of nodes yield highly accurate results. A review of various numerical calculations of three-dimensional lattice sums is given in Ref. [85].*

5.6.2

Method of Functional Equations

In this section, we describe the method of functional equations in the class of analytical functions [16,80,86–90,94]. This method is used for solution of boundary value problems for the Laplace equation.

Let us consider the method of functional equations in the example of a solution of the following problem. Consider the cell $Q_{(0,0)}$ with N nonoverlapping circular disks D_k of radius r with the centers $a_k \in Q_{(0,0)}$ ($k = 1, 2, \dots, N$). Let D_0 be the complement of the closure of all disks D_k to $Q_{(0,0)}$. We study the conductivity of the doubly periodic composite material when the domains $D_{per} := \bigcup_{(m_1, m_2)} (D_0 \cup \partial Q_{(0,0)} + m_1 \omega_1 + m_2 \omega_2)$ and $D_k + m_1 \omega_1 + m_2 \omega_2$ (m_1, m_2 are integers) are occupied by materials of conductivities λ_0 and λ , respectively. The conductivity of the inclusions λ is expressed relative to λ_0 . Hence, the conductivity of the matrix can be taken as unity ($\lambda_0 = 1$). The local potential $T(z)$ in $Q_{(0,0)}$ satisfies the conjugation conditions:

$$\begin{aligned} T^+(t) &= T^-(t), \quad \frac{\partial T^+}{\partial n}(t) = \lambda \frac{\partial T^-}{\partial n}(t) \quad \text{on } \partial D_k = \{t \in \mathbb{C} : |t - a_k| = r\}, \\ k &= 1, 2, \dots, N \end{aligned} \quad (5.120)$$

The potential $T(z)$ satisfies the quasi-periodicity conditions:

$$T(z + \omega_1) = T(z) + \Omega_1, \quad T(z + \omega_2) = T(z) + \Omega_2 \quad (5.121)$$

Here, the function $T(z)$ is harmonic in $Q_{(0,0)}$ except ∂D_k ($k = 1, 2, \dots, N$), the circles ∂D_k are orientated in the clockwise direction. In order to determine the effective conductivity tensor Λ , it is sufficiently to solve the problem (5.120), (5.121) with two linear independent vectors (Ω_1, Ω_2) . The problem (5.120) is reduced to the $\mathbb{R}$ -linear conjugation problem (see Section 5.2.4). For simplicity, consider the case $N = 1$:

$$\psi(t) = \psi_1(t) + \rho \left(\frac{r}{t-a} \right)^2 \overline{\psi_1(t)} - 1, \quad |t-a| = r \quad (5.122)$$

The unknown function $\psi(z)$ can be presented in the form of its Taylor expansion: $\psi(z) = \rho \sum_{l=0}^{\infty} \psi_l (z-a)^l$. The problem (5.122) is reduced to the following functional

equation:

$$\psi(z) = \rho \sum_{l=0}^{\infty} \overline{\psi_l} r^{2(l+1)} \{E_{l+2}(z-a) - (z-a)^{-(l+2)}\} + 1, \quad |z-a| \leq r \quad (5.123)$$

We look for $\psi(z)$ in the form of the series expansion in r^2 : $\psi(z) = \sum_{s=0}^{\infty} r^{2s} \psi^{(s)}(z)$. The functional Eq. (5.123) has a unique solution which can be found by the method of successive approximation uniformly convergent in $|z-a| \leq r$:

$$\begin{aligned} \psi^{(0)}(z) &= 1, \\ \psi^{(p+1)}(z) &= \rho [\overline{\psi_p^{(0)}} \eta_{p+2}(z-a) + \overline{\psi_{p-1}^{(1)}} \eta_{p+1}(z-a) + \dots + \overline{\psi_0^{(p)}} \eta_2(z-a)] \end{aligned} \quad (5.124)$$

where $\eta_p(z) = E_p(z) - z^{-p}$. Using Eqs. (5.50) and (5.124), Rylko [81] calculated approximately $\hat{\lambda}$ for a square array of cylinders and $\rho = 1$:

$$\hat{\lambda} = \frac{1+v}{1-v} + 6S_4^2 \pi^{-4} \frac{v^5}{(1-v)^2} + 2(9S_4^2 + 7S_8^2) \pi^{-8} v^9 + O(v^{10}) \quad (5.125)$$

where $v = \frac{N\pi r^2}{|Q_{(0,0)}|}$ is the concentration of the disks in the cell $Q_{(0,0)}$, $|Q_{(0,0)}|$ is the area of $Q_{(0,0)}$, $S_2 = \pi$, $S_4 \approx 3.1512112$, $S_8 \approx 4.2557732$. The first term in Eq. (5.125) corresponds to the CMA (5.54). More complicated investigation of the functional Eq. (5.123) implies the following exact formula for a square array:

$$\begin{aligned} \hat{\lambda} &= 1 + 2\rho v + 2\rho^2 v^2 \\ &+ 2\rho^2 v^2 \frac{1}{\pi} \sum_{k=1}^{\infty} \rho^k \sum_{m_1=1}^{\infty} \sum_{m_2=1}^{\infty} \dots \sum_{m_k=1}^{\infty} \sigma_{m_1}^{(1)} \sigma_{m_2}^{(m_1)} \dots \sigma_{m_k}^{(m_{k-1})} \sigma_1^{(m_k)} \left(\frac{v}{\pi}\right)^{2(m_1+m_2+\dots+m_k)-k} \end{aligned} \quad (5.126)$$

where $\sigma_k^{(n)}$ has the form (5.115).

Similar arguments can be applied to the general $\mathbb{R}$ -linear conjugation problem with arbitrary N . The effective conductivity tensor $\hat{\Lambda}$ has the following structure:

$$\hat{\Lambda} = (1 + 2\rho v) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2\rho v \sum_{k=1}^{\infty} \begin{pmatrix} \operatorname{Re} A_k & \operatorname{Im} A_k \\ \operatorname{Im} A_k & C_k \end{pmatrix} v^k \quad (5.127)$$

where

$$A_k = |Q_{(0,0)}|^k \sum_{n_1 \dots n_p} B_{n_1 \dots n_p}^{(k)} e_{n_1 \dots n_p}(\omega_1, \omega_2) \quad (5.128)$$

The constants $B_{n_1 \dots n_p}^{(k)}$ depend only on k , ρ and $n_1, \dots, n_p$. Here, $n_j = 2, 3, \dots$; $k = 1, 2, \dots$. The values C_k have an analogous form. Only the terms $e_{n_1 \dots n_p}(\omega_1, \omega_2)$ defined by (5.117) depend on the centers of inclusions a_k in the representation (5.127) of $\hat{\Lambda}$. The first few coefficients A_k have the form [86,98]

$$\begin{aligned}
 A_1 &= \frac{\rho}{\pi} e_2, \quad A_2 = \frac{\rho^2}{\pi^2} e_{22}, \quad A_3 = \frac{1}{\pi^3} [-2\rho^2 e_{33} + \rho^3 e_{222}] \\
 A_4 &= \frac{1}{\pi^4} [3\rho^2 e_{44} - 2\rho^3 (e_{332} + e_{233}) + \rho^4 e_{2222}] \\
 A_5 &= \frac{1}{\pi^5} [-4\rho^2 e_{55} + \rho^3 (3e_{442} + 6e_{343} + 3e_{244}) \\
 &\quad - 2\rho^4 (e_{3322} + e_{2332} + e_{2233}) + \rho^5 e_{22222}] \\
 A_6 &= \frac{1}{\pi^6} [5\rho^2 e_{66} - 4\rho^3 (e_{255} + 3e_{354} + 3e_{453} + e_{552}) \\
 &\quad + \rho^4 (3e_{2244} + 6e_{2343} + 4e_{3333} + 3e_{2442} + 6e_{3432} + 3e_{4422}) \\
 &\quad - 2\rho^5 (e_{22233} + e_{22332} + e_{23322} + e_{33222} + \rho^6 e_{222222})]
 \end{aligned} \tag{5.129}$$

where the argument (ω_1, ω_2) is omitted. In particular, for macroscopically isotropic composites (5.127) becomes

$$\hat{\lambda} = 1 + 2\rho v + 2\rho v \sum_{k=1}^{\infty} A_k v^k \tag{5.130}$$

5.7 Representative Cell

One of the most important notation of composites and porous media is the *representative volume element* (RVE) or *representative cell* already used in this chapter. One can give a vague physical definition of this term as follows. RVE is a part of material which is small enough from a macroscopic point of view that it can be treated as a typical element of the heterogeneous medium. On the other hand, it is sufficiently large in the microscopic scale that it represents a typical microstructure of the material under consideration. In the present section following Ref. [91], we first give a rigorous definition of the representative element and then determine its minimal size. The geometrical interpretation of the problem is shown in Figure 5.3. The large cell Q' presented in Figure 5.3a is replaced by a smaller one, Q (see Figure 5.3b) with three inclusions per periodic cell.

Note that Adler and co-workers [5,6] discussed questions of the reconstruction of porous media by statistical data and a numerically constructed RVE.

Consider a two-dimensional two-component periodic composite medium made from a collection of nonoverlapping identical circular disks embedded in an otherwise uniform matrix. Let the inclusions have scalar conductivity λ and be separated by a matrix of unit conductivity. Let $\rho = (\lambda - 1)/(\lambda + 1)$ be the contrast parameter. It is

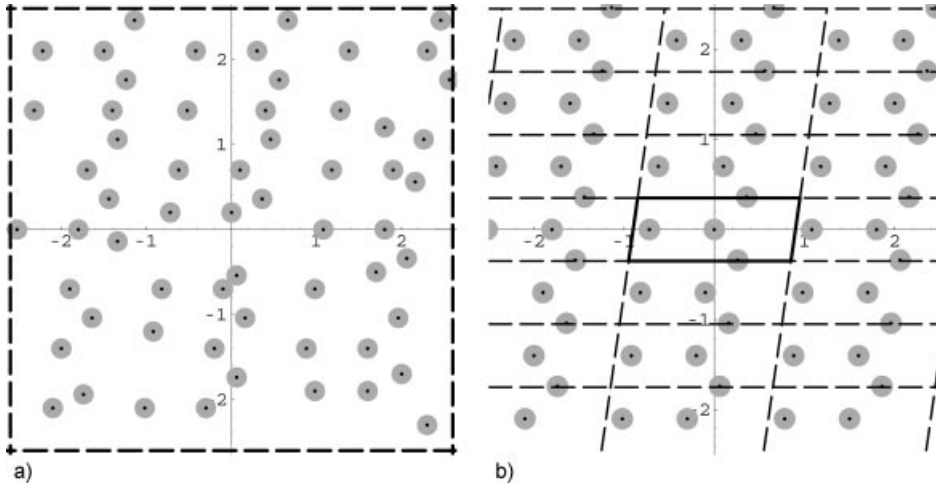


Figure 5.3 Representative cells.

established in Section 5.6.2 that the effective conductivity tensor $\hat{\Lambda}$ has the form of a double series in the concentration of inclusions and on “basic elements” which depend only on locations of the inclusions (see Eqs. (5.127) and (5.128)). These basic elements are written in terms of the Eisenstein series. Coefficients in the double series depend on ρ . We say that two composites are equivalent if expansions of their $\hat{\Lambda}$ have the same basic elements. Therefore, we divide the set of the composites with circular identical inclusions into classes of equivalence determined only by geometrical structure of the composite. In particular, composites with the same locations of inclusions but with different ρ belong to the same class of equivalence. Note that composites belonging to a class of equivalence can have different $\hat{\Lambda}$; and composites from different classes can have the same $\hat{\Lambda}$. Each composite material is represented by a periodic cell. In each class of equivalence, we choose a composite having the minimal size cell. This cell is called *the representative cell* of the considered class of equivalent composite materials.

We propose a constructive algorithm to determine the representative cell for any distribution of inclusions using only pure geometrical parameters. More precisely, at the beginning, we calculate the generalized Eisenstein–Rayleigh sums (5.117) depending on the centers of circular inclusions for given large cell. Then using these sums, we construct the (minimal) representative cell, i.e. we calculate its fundamental translation vectors and determine the positions of inclusions within this cell.

Consider a large fundamental region Q' constructed by the fundamental translation vectors ω'_1 and ω'_2 . Let Q' contain N' non-overlapping circular disks D'_k of radius r with the centers $a'_k \in Q'$ ($k = 1, 2, \dots, N'$). Let $\hat{\Lambda}'$ be the effective conductivity tensor of the composite material represented by the region Q' with inclusions D'_k . We are interested in the following question. To replace Q' by another small cell Q which contains inclusions $D_k = \{z \in \mathbb{C} : |z - a_k| < r\}$ ($k = 1, 2, \dots, N$) and which has an

effective conductivity tensor $\hat{\Lambda}$ close to $\hat{\Lambda}'$. We assume that the concentration v of the inclusions in both materials is the same. Closeness is defined by the accuracy $O(v^{L+1})$ for the difference $\Delta\hat{\Lambda} = \hat{\Lambda} - \hat{\Lambda}'$ with prescribed L . We say that Q is a representative cell for the region Q' with the accuracy $O(v^{L+1})$ if $\Delta\hat{\Lambda} = O(v^{L+1})$. We say that Q is the minimal representative cell for the region Q' if Q is a representative cell with minimal possible area $|Q|$. For brevity, we further call the minimal representative cell the representative cell. The existence of the representative cell is evident since in the worst case one can take $Q = Q'$.

We adopt the designations generalized Eisenstein-Rayleigh sums for the representative cell. Consider Eq. (5.127) for the large cell Q'

$$\hat{\Lambda}' = (1 + 2\rho v) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2\rho v \sum_{k=1}^{\infty} \begin{pmatrix} \text{Re} A'_k & \text{Im} A'_k \\ \text{Im} A'_k & C'_k \end{pmatrix} v^k \quad (5.131)$$

$$A'_k = |Q'|^k \sum_{n_1 \dots n_p} B_{n_1 \dots n_p}^{(k)} e_{n_1 \dots n_p}(\omega'_1, \omega'_2) \quad (5.132)$$

Note that the coefficients $B_{n_1 \dots n_p}^{(k)}$ have the same form in Eqs. (5.128) and (5.131). $\Delta\hat{\Lambda}$ is of order $O(v^{L+1})$ if $A'_k = A_k$ for $k = 1, 2, \dots, L-1$. Therefore, $\Delta\hat{\Lambda}$ is of order $O(v^{L+1})$ if and only if

$$|Q'|^k e_{n_1 \dots n_p}(\omega_1, \omega_2) = |Q'|^k e_{n_1 \dots n_p}(\omega'_1, \omega'_2) \quad (5.133)$$

for $k = 1, 2, \dots, L-1$ and corresponding sets of the numbers $n_1, \dots, n_p$. According to our definition, Q is a representative cell for the region Q' with the accuracy $O(v^{L+1})$ if and only if the relations Eq. (5.132) are fulfilled.

One can consider Eq. (5.132) as a system of equations with respect to $\omega_1, \omega_2, a_1, a_2, \dots, a_N$ including the unknown number N with the restriction $|a_j - a_m| \leq 2r$ ($j \neq m$). One can assume that one of the centers, say a_N , lies at the origin, since geometrically any cell is determined up to translation. The fundamental region Q as well as the translation vectors ω_1, ω_2 can be chosen in infinitely many ways [74]. For any doubly periodic structure on the plane, it is always possible to construct such a pair ω_1, ω_2 that $\omega_1 > 0$ and $\text{Im}\tau > 0$.

The area of Q is calculated by ω_1 and ω_2

$$|Q| = \omega_1^2 \text{Im}\tau \quad (5.134)$$

On the other hand, we also have $|Q| = \frac{N\pi r^2}{v}$ that yields the formula

$$\omega_1 = \sqrt{\frac{N\pi r^2}{v \text{Im}\tau}} \quad (5.135)$$

In order to construct the representative cell with the prescribed accuracy $O(v^{L+1})$, we propose to solve the system (5.132) with fixed L increasing the number of inclusions in the cell N from 1 to N' . Then, N is fixed in each step of the study of Eq. (5.132).

Applying Eqs. (5.119) and (5.133), we rewrite Eq. (5.132) in the form

$$(\text{Im}\tau)^k e_{n_1, \dots, n_p}(1, \tau) = |Q'|^k e_{n_1, \dots, n_p}(\omega'_1, \omega'_2), \quad k = 1, 2, \dots, L-1 \quad (5.136)$$

We can consider Eq. (5.135) as a system with respect to τ , $a_1, a_2, \dots, a_{N-1}$ ($a_N = 0$) with the restriction $|a_j - a_m| \geq 2r$ ($j \neq m$). The right-hand part of Eq. (5.135) is known. If we know a solution of Eq. (5.135), we can calculate ω_1 from Eq. (5.134).

It is also possible to state the problem of the representative cell with prescribed form of the cell Q . Let us consider the case when Q is a rectangle. Then, $\tau = i\alpha$, where α is positive and Eq. (5.134) implies that

$$\omega_1 = \sqrt{\frac{N\pi r^2}{\alpha v}} \quad (5.137)$$

Equations (5.135) become

$$\alpha^k e_{n_1, \dots, n_p}(1, i\alpha) = |Q'|^k e_{n_1, \dots, n_p}(\omega'_1, \omega'_2), \quad k = 1, 2, \dots, L-1 \quad (5.138)$$

Numerical examples of solution to Eqs. (5.135) and (5.137) are presented in Ref. [91]. One can also find there a discussion devoted to other shapes of inclusions.

A spatial theory of the representative elements can also be constructed due to Berdichevskij's 3D analogs of the elliptic functions (see Remark 5.6.2).

5.8

Nonlinear Heat Conduction

In the general mathematical theory of the nonlinear behavior of materials, the conductivity (for instance, electric) depends locally on the gradient of the potential. However, in the thermal conductivity, we have another dependence. Namely, the local coefficient depends on the potential, i.e. on the temperature distribution. Then, Fourier's law (5.1) becomes

$$\mathbf{q} = -\lambda(T)\nabla T \quad (5.139)$$

This case is easier to study due to the transformation (5.1.3) from Ref. [16, Chapter V].

There is a wonderful result in the nonlinear homogenization theory due to Artola and Duvaut [92] (see also Ref. [93]) devoted to homogenization of Eq. (5.138). It follows from Ref. [92] that in order to obtain a formula for the effective conductivity, it is sufficient to take a formula from linear theory with constant λ and to substitute $\lambda(T)$ instead of this constant. For instance, in the linear case, $\hat{\Lambda}$ for laminates is determined by Eqs. (5.44) and (5.52). Let the conductivities of the constituents depend on T , i.e. $\lambda_j = \lambda_j(T)$ ($j=1, 2$). Then, the effective conductivities in this nonlinear case are exactly calculated by the same formulas (5.44) and (5.52) but with replacing $\hat{\lambda}_j$ and λ_j by the functions $\hat{\lambda}_j(T)$ and $\lambda_j(T)$.

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6

Modeling of Composite Heat Transfer in Open-Cellular Porous Materials at High Temperatures*

Kouichi Kamiuto

6.1

Introduction

Open-cellular porous materials (or open-cell foams) consist of three-dimensional dodecahedron-like cells with pentagonal or hexagonal open-cell walls [1], as shown in Figure 6.1a, where a pentagonal dodecahedron cell is illustrated as a typical example, and are characterized by some prominent physical properties such as high porosity (0.8–0.95), low pressure drop, large volumetric heat transfer coefficient (10^4 – $10^7 \text{ W m}^{-3} \text{ K}^{-1}$) and large radiation extinction coefficient (10^2 – 10^3 m^{-1}). So far, this kind of porous medium has been widely utilized as filters, thermal insulators, sound absorbers, electrodes, impact energy absorbers, and so on. In addition to these traditional applications, innovative technological applications for high-temperature heat transfer augmentation, lean-combustion enhancement and waste heat recovery from various furnaces have been proposed during recent decades [2–8], and a number of practical equipments using open-cellular porous materials have been developed, particularly, in relation to the saving and effective use of energy in metallurgical and petrochemical industries [3,5,8].

Obviously, thermal design and operation of these equipments require qualitative knowledge of fluid flow and heat transfer characteristics of open-cellular porous media to be known. The aim of the present chapter is twofold: first, to establish predictive models for qualitatively describing the thermal, radiative and fluid mechanical processes in open-cellular porous materials; and second, to apply these models to predictions of pure radiative heat transfer, combined conductive and radiative heat transfer and combined forced-convective and radiative heat transfer in open-cell forms at high temperatures.

* Please find the nomenclature at the end of this chapter.

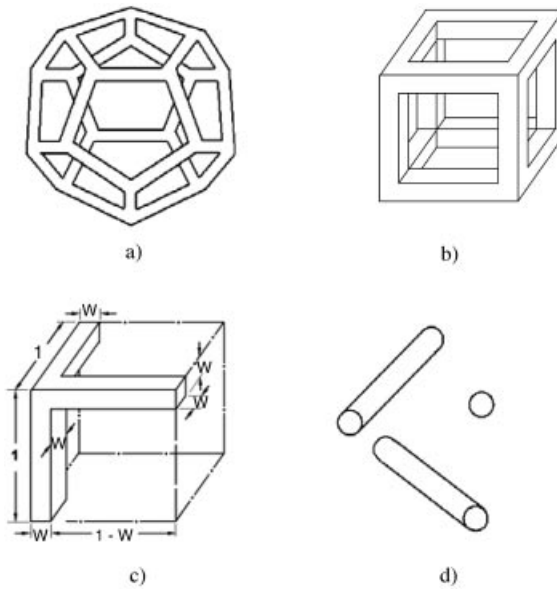


Figure 6.1 Model systems for open-cellular porous materials: (a) perspective view (case of a pentagonal dodecahedron cell); (b) unit cell model of Dul'nev; (c) rearranged unit cell model; (d) equivalent scatterers derived from the unit cell model.

6.2

Governing Equations

The conservation equations of mass, momentum and energy in porous media have been rigorously derived by several authors using a local volume-averaging technique of Whitaker [9], but the obtained expressions contain a number of parameters that are difficult to estimate, and must be determined experimentally. For this reason, we begin with semi-empirical or heuristic governing equations for describing turbulent transport processes in porous media [7,10,11].

The major assumptions are as follows: (a) flow field is in a turbulent state, but the Mach number is much less than unity; (b) effects of buoyancy, hydrodynamic dispersion, viscous dissipation and thermal expansion are negligible; and (c) the porosity is uniform within a porous medium.

Under these assumptions, the conservation equations of mass and momentum for turbulent forced-convection flow are written as follows:

$$\nabla \cdot \mathbf{V} = 0 \quad (6.1)$$

$$\rho_f \left[\frac{\partial \mathbf{V}}{\partial t} + \{ \nabla \cdot (\mathbf{V} \mathbf{V}) \} / \phi \right] = -\nabla P + \mu_f \nabla^2 \mathbf{V} - \phi \left(\frac{\mu_f}{K} + \frac{\rho_f F}{\sqrt{K}} |\mathbf{V}| \right) \mathbf{V} \quad (6.2)$$

where $\mathbf{V}$ is the Darcian velocity vector, K is the permeability and F is the Forchheimer coefficient. In Eq. (6.2), we represent the Forchheimer term in the form of $|\mathbf{V}|\mathbf{V}$ for a two- or three-dimensional flow in a porous medium in accordance with Stanek and Szekely [12], but it should be noted that this expression has not yet been experimentally verified. If there is an appreciable temperature difference between the fluid and solid phases within a porous medium, the local thermal equilibrium assumption cannot be justified, and a two-temperature model should be introduced for the energy equation. When the phase volume-averaged temperatures for the fluid and solid phases are represented by T_f and T_s , the energy equations may be written as

$$\phi(\rho C_p)_f \frac{\partial T_f}{\partial t} + (\rho C_p)_f \mathbf{V} \cdot \nabla T_f = \nabla \cdot \left\{ \left(\underline{\mathbf{K}}_{cf} + \underline{\mathbf{K}}_d \right) \cdot \nabla T_f \right\} - h_v(T_f - T_s) \quad (6.3)$$

$$(1-\phi)(\rho C_p)_s \frac{\partial T_s}{\partial t} = \nabla \cdot \left(\underline{\mathbf{K}}_{cs} \cdot \nabla T_s \right) - h_v(T_s - T_f) - \text{div} \mathbf{q}_R \quad (6.4)$$

$$\text{div} \mathbf{q}_R = \int_0^\infty \sigma_{av} (4\pi I_{bv} - G_v) dv \quad (6.5)$$

where $\underline{\mathbf{K}}_{cf}$ and $\underline{\mathbf{K}}_{cs}$, respectively, represent the effective thermal conductivity tensors for the fluid and solid phases, $\underline{\mathbf{K}}_d$ is the thermal dispersion tensor, h_v is the volumetric heat transfer coefficient between the fluid and solid phases, and G_v represents the spectral incident radiation defined by $\int_{4\pi} I_v(\mathbf{r}, \Omega) d\Omega$. Here, $I_v(\mathbf{r}, \Omega)$ is the spectral intensity of radiation.

If both the fluid and solid phases are in local thermal equilibrium, then the use of the one-temperature model may be fully justified:

$$(\rho C_p)_m \frac{\partial T}{\partial t} + (\rho C_p)_f \mathbf{V} \cdot \nabla T = \nabla \cdot \left\{ \left(\underline{\mathbf{K}}_{eff} + \underline{\mathbf{K}}_d \right) \cdot \nabla T \right\} - \text{div} \mathbf{q} \quad (6.6)$$

$$(\rho C_p)_m = \phi(\rho C_p)_f + (1-\phi)(\rho C_p)_s \quad (6.7)$$

where $\underline{\mathbf{K}}_{eff}$ represents the stagnant effective thermal conductivity tensor for a porous medium. As can be seen from Eqs. (6.4)–(6.6), the energy equations involve the incident radiation G_v , and thus this quantity must be evaluated by solving the equation of transfer.

For a plane-parallel system, the spectral equation of transfer is written as

$$\mu \frac{\partial I_v(y, \mu)}{\partial y} + \beta_v I_v(y, \mu) = (1-\omega_v)\beta_v I_{bv}(y) + \frac{\omega_v \beta_v}{2} \int_{-1}^1 I_v(y, \mu') P_v(\mu, \mu') d\mu' \quad (6.8)$$

The boundary conditions for opaque diffuse boundaries are

$$\left. \begin{aligned} I_v(0, \mu > 0) &= \varepsilon_{1v} I_{bv}(0) + 2(1 - \varepsilon_{1v}) \int_0^1 I_v(0, -\mu') \mu' d\mu' \\ I_v(\gamma_0, -\mu) &= \varepsilon_{2v} I_{bv}(\gamma_0) + 2(1 - \varepsilon_{2v}) \int_0^1 I_v(\gamma_0, \mu') \mu' d\mu' \end{aligned} \right\} \quad (6.9)$$

For gray media, the equation of transfer and its associated boundary conditions are given as follows:

$$\mu \frac{\partial I(\gamma, \mu)}{\partial \gamma} + \beta I(\gamma, \mu) = (1 - \omega) \beta \frac{\sigma T^4(\gamma)}{\pi} + \frac{\omega \beta}{2} \int_{-1}^1 I(\gamma, \mu') P(\mu, \mu') d\mu' \quad (6.10)$$

$$\left. \begin{aligned} I(0, \mu > 0) &= \varepsilon_1 \frac{\sigma T^4(0)}{\pi} + 2(1 - \varepsilon_1) \int_0^1 I(0, -\mu') \mu' d\mu' \\ I(\gamma_0, -\mu) &= \varepsilon_2 \frac{\sigma T^4(\gamma_0)}{\pi} + 2(1 - \varepsilon_2) \int_0^1 I(\gamma_0, \mu') \mu' d\mu' \end{aligned} \right\} \quad (6.11)$$

Instead of the exact equation of transfer, the first-order spherical harmonic approximation to the equation of transfer called the P_1 approximation has been often utilized because only the incident radiation and radiative heat flux in a medium are required for analyses of composite heat transfer and just the P_1 approximation yields the governing equations with respect to these quantities. Moreover, the gray approximation to the radiative properties is often adopted.

The gray P_1 equations in a plane-parallel system are

$$\left. \begin{aligned} \frac{dG}{d\gamma} + 3\beta(1 - \omega \tilde{g}) q_R &= 0 \\ \frac{dq_R}{d\gamma} + \beta(1 - \omega) G &= 4\beta(1 - \omega) \sigma T^4 \end{aligned} \right\} \quad (6.12)$$

The boundary conditions for gray opaque diffuse boundaries are appropriately given by the following Marshak ones:

$$\left. \begin{aligned} \gamma = 0 : \quad \varepsilon_1 G(0) + 2(2 - \varepsilon_1) q_R(0) &= 4\varepsilon_1 \sigma T_1^4 \\ \gamma = \gamma_0 : \quad \varepsilon_2 G(\gamma_0) - 2(2 - \varepsilon_2) q_R(\gamma_0) &= 4\varepsilon_2 \sigma T_2^4 \end{aligned} \right\} \quad (6.13)$$

6.3

Transport Properties and Heat Transfer Correlation

6.3.1

Effective Thermal Conductivities

For isotropic porous media such as open-cell foams, $\underline{\mathbf{K}}_{cf}$, $\underline{\mathbf{K}}_{cs}$ and $\underline{\mathbf{K}}_{eff}$ generally become second-rank tensors and may be represented in the following form:

$$\underline{\underline{K}}_{cf} = k_{cf} \underline{\underline{I}} \quad (6.14)$$

$$\underline{\underline{K}}_{cs} = k_{cs} \underline{\underline{I}} \quad (6.15)$$

$$\underline{\underline{K}}_{eff} = k_{eff,c} \underline{\underline{I}} \quad (6.16)$$

where $\underline{\underline{I}}$ denotes the unit tensor.

Parameters k_{cf} , k_{cs} and $k_{eff,c}$ are scalar quantities and represent effective thermal conductivities of the fluid and solid phases and a porous medium, respectively.

Several empirical or semi-theoretical models are proposed for the effective thermal conductivity of an open-cell foam. In what follows, we refer to some representative models.

Dul'nev [13] regarded interconnected porous materials as an assembly of cubic unit cells, as shown in Figure 6.1b and c, and derived the following theoretical formula:

$$k_{eff,c}/k_f = (k_s/k_f)w^2 + (1-w)^2 + \frac{2(1-w)w(k_s/k_f)}{(1-w)(k_s/k_f) + w} \quad (6.17)$$

$$w = \frac{1}{2} + \cos \left[\frac{1}{3} \cos^{-1}(2\phi - 1) + \frac{4}{3}\pi \right] \quad (6.18)$$

As understood from Eq. (6.17), Dul'nev's formula involves an interaction term between the fluid and solid phases, and cannot be applied to a two-temperature energy equation model. The accuracy of Dul'nev's formula is addressed in comparison with available experimental data. Results are shown in Figure 6.2, indicating that Dul'nev's formula reproduces 87.03% of available data with an accuracy of less than $\pm 30\%$.

Bhattacharya *et al.* [14] proposed an empirical correlation of $k_{eff,c}$ by combining two limiting expressions of the effective thermal conductivity of an open-cell form:

$$k_{eff,c}/k_f = A\{\phi + (1-\phi)/(k_s/k_f)\} + (1-A)/\{\phi + (1-\phi)/(k_s/k_f)\} \quad (6.19)$$

Here, the former represents the upper limit with the solid and fluid phases arranged in parallel to the direction to the heat flow path, while the latter corresponds to the lower limit with the two phases arranged in series.

Moreover, A is an adjustable parameter and the best fit for their experimental data was found for $A = 0.35$. Results of a comparison between model predictions based on Eq. (6.19) and available experimental data show that Eq. (6.19) reproduces 87.03% of the data within an accuracy of $\pm 30\%$, which surprisingly coincides with that of Dul'nev's formula. For this reason, we skip graphical representation of the parity plot comparing the model predictions and the experimental data.

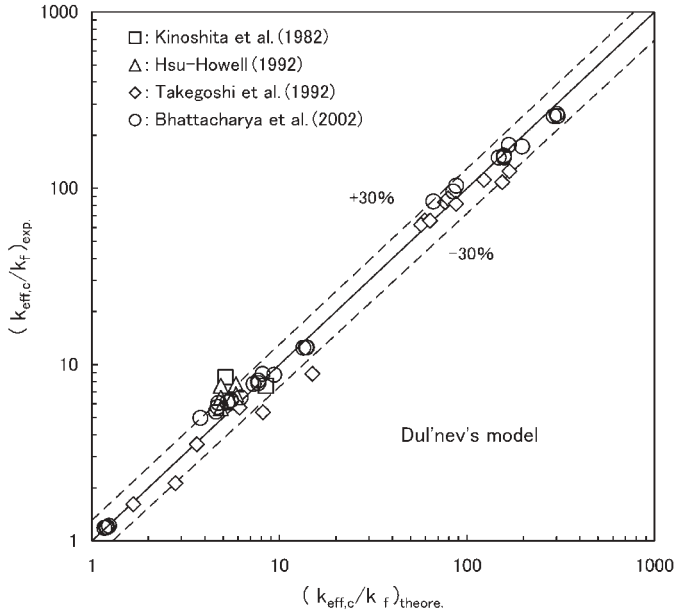


Figure 6.2 Correlation between theoretical values of $k_{\text{eff},c}$ computed from Dul'nev's formula and experimental values of $k_{\text{eff},c}$.

Schuetz and Glicksman [15] derived a semi-theoretical correlation of an isotropic open-cell foam on the basis of the “in-line cubes with 100% struts” model:

$$k_{\text{eff},c}/k_f = \phi + \frac{1}{3}(1-\phi)(k_s/k_f) \quad (6.20)$$

The first term of the right-hand side represents the contribution of the fluid phase, which was assumed to be unity in the original model. A numerical factor $1/3$ in the second term was introduced to take into account the fact that one-third of the struts are oriented in the heat flow direction. The Schuetz–Glicksman model can be readily incorporated into the two-temperature model because, as seen from Eq. (6.20), $k_{\text{eff},c}$ consists of two terms corresponding to the fluid and solid phases, respectively. Comparison between model predictions and the existing experimental data is shown in Figure 6.3. The Schuetz–Glicksman model approximates 88.9% of the data within an accuracy of $\pm 30\%$ and is more accurate than the Dul'nev and Bhattacharya–Calmidi–Mahajan models. From the present comparison results, the Schuetz–Glicksman model is recommended as a suitable model for $k_{\text{eff},c}$. If this model is selected for the expression of $k_{\text{eff},c}$ then it is reasonable to express k_{cf} and k_{cs} in the following form:

$$k_{\text{cf}} = \phi k_f \quad (6.21)$$

$$k_{\text{cs}} = (1-\phi)k_s/3 \quad (6.22)$$

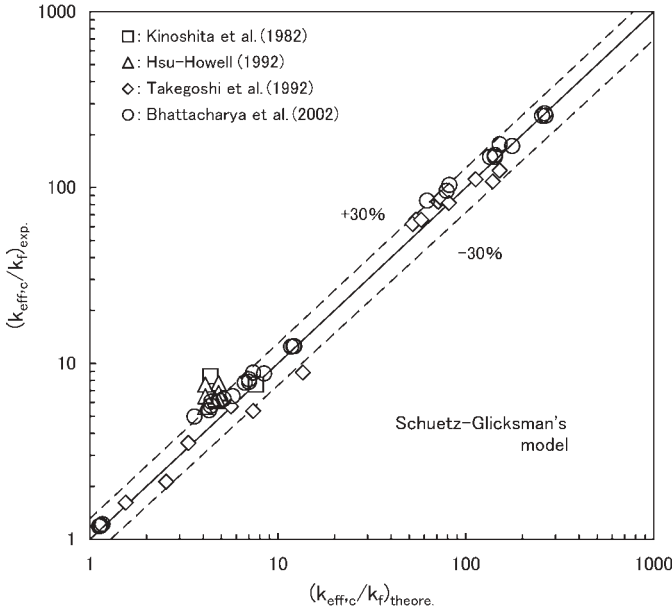


Figure 6.3 Correlation between theoretical values of $k_{eff,c}$ computed from the Schuetz–Glicksman formula and experimental values of $k_{eff,c}$.

6.3.2

Thermal Dispersion Conductivities

When fluid flows through an open-cell foam, lateral and axial mixings of fluid occur from a unit cell to the neighboring cells through openings of a cell. If a temperature gradient exists within a porous medium, these processes cause net heat transport called thermal dispersion. For open-cellular porous materials, the dispersion conductivity tensor becomes a second-rank tensor with zero off-diagonal elements and may be written as

$$\underline{\underline{K}}_d = \mathbf{nn}k_{dl} + (\underline{\underline{I}} - \mathbf{nn})k_{da} \quad (6.23)$$

where k_{dl} and k_{da} , respectively, represent the lateral and axial components of the diagonal term of $\underline{\underline{K}}_d$ and $\mathbf{n}$ is the unit vector perpendicular to a flow direction. As for k_{dl} , Koch and Brady [16] proposed the following expression:

$$k_{dl} = \rho_f C_{pf} \gamma_{dl} \sqrt{K} u = \gamma_{dl} \text{Pr} \left(u \sqrt{K} / \nu_f \right) k_f \quad (6.24)$$

where γ_{dl} is the lateral dispersion coefficient and K the permeability.

Hunt and Tien [17] found that a value of γ_{dl} is about 0.025 for a porosity of 0.97. Although γ_{dl} should be a function of porosity, its functional relationship has not yet

been experimentally established. However, on the basis of the theoretical results of Koch and Brady, Hunt and Tien suggested the following equation:

$$\gamma_{dl} = 0.0877 / |\ln(1-\phi)| \quad (6.25)$$

As for k_{da} , Kamiuto and Yee [18] gave the following expression similar to Eq. (6.24):

$$\begin{aligned} k_{da} &= \rho_f C_{pf} \gamma_{da} \sqrt{K} u \\ &= \gamma_{da} \text{Pr} \left(u \sqrt{K} / \nu_f \right) k_f \end{aligned} \quad (6.26)$$

where γ_{da} is the axial dispersion coefficient and can be represented by

$$\gamma_{da} = 9.269 + 2005.4(\phi - 0.8) - 16330(\phi - 0.8)^2 \quad (6.27)$$

Figure 6.4 shows predicted values of k_{da}/k_f based on Eqs. (6.26) and (6.27) and experimental data [19]. Comparison of γ_{da} with γ_{dl} reveals that a value of γ_{da} is about 1200 times greater than that of γ_{dl} , although the expression for γ_{dl} was obtained using the experimentally determined radial thermal dispersion coefficients of fibrous media with ϕ greater than 0.94 and should be carefully treated in extrapolating it to porous media with ϕ less than about 0.9. Moreover, it should be noted that experimentally determined thermal dispersion conductivities contain effects of turbulence because, in experiments as for thermal dispersion, the contribution of the thermal dispersion cannot be separated from that of turbulence and therefore, as

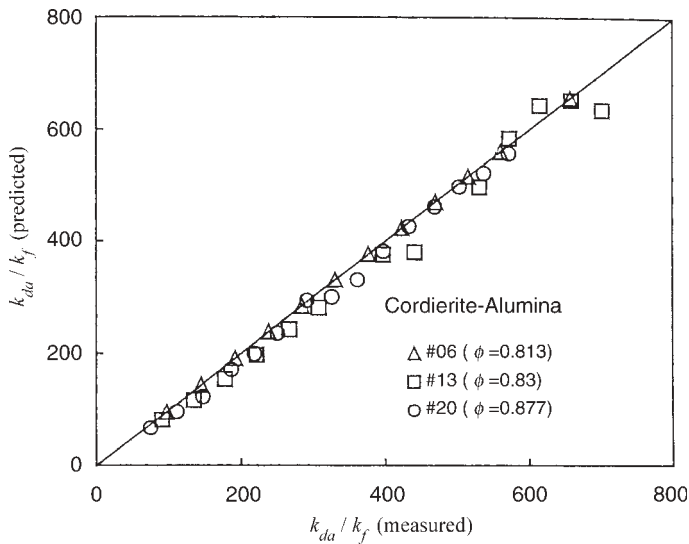


Figure 6.4 Predicted versus measured values of the dimensionless axial dispersion conductivity k_{da}/k_f .

pointed out by Yee and Kamiuto [20], the experimentally determined so-called dispersion coefficients involve both contributions.

6.3.3

Radiative Properties

Radiative properties needed for radiative transfer calculations in participating media are the extinction coefficient β , albedo ω and scattering phase function.

Several attempts to model the radiative properties of complex open-cellular porous media have been made. Hsu and Howell [21] presented a semi-empirical formula of the effective extinction coefficient β (m^{-1}) as a function of actual pore size D_m (m):

$$\beta = 3(1-\phi)/D_m \quad (6.28)$$

They claimed that Eq. (6.28) is applicable to the open-cell forms with pore diameter greater than 6×10^{-4} (m).

Doermann and Sacadura [22] proposed a sophisticated models for the extinction coefficient, albedo and phase function of an open-cell foam on the basis of geometrical optics and diffraction theory, but they did not compare their model predictions with experimental data.

Kamiuto [23] derived analytical formula for the radiative properties of an open-cellular porous medium by decomposing a Dul'nev unit cell into two cylindrical struts and one spherical strut juncture (Figure 6.1b) and by applying geometrical optics and diffraction theory to these scatterers which are assumed to be randomly oriented in space. Note that there exist three struts in a unit cell but only two are effective in the radiation process because the vertical strut is located in the shadow region of the strut juncture, when thermal radiation is normally incident on the upper surface of the unit cell, and thus does not interact with incident thermal radiation. There exist two kinds of radiative properties, depending on the way of dealing with the effect of diffraction in the equation of transfer: scaled and unscaled radiative properties. The former appears in the equation of transfer where the diffraction scattering phase function is eliminated utilizing Dirac's delta function; the latter is obtained from the equation of transfer where the effect of diffraction is left untouched. The unscaled radiative properties are given by

$$\beta = \frac{\pi}{2} \left[(6/\pi)^{2/3} w^2 + \frac{4w}{\sqrt{\pi}} (1-w) \right] / D_c \quad (6.29)$$

$$\omega = \sigma_s / \beta = (1 + \rho_H) / 2 \quad (6.30)$$

$$\tilde{g} = \frac{1}{2} \int_{-1}^1 P(\mu') \mu' d\mu' = (1 + \rho_H \tilde{g}_d) / (1 + \rho_H) \quad (6.31)$$

where D_c is a mean size of the Dulnev unit cells, ρ_H is the hemispherical reflectivity of struts and strut junctures and $\tilde{g}_d$ is the asymmetry factor of the

surface-scattering phase function of a diffuse sphere, i.e. $-4/9$. The scaled radiative properties are

$$\beta^* = \beta/2 \quad (6.32)$$

$$\omega^* = \rho_H \quad (6.33)$$

$$\tilde{g}^* = \tilde{g}_d \quad (6.34)$$

Moreover, the scattering phase function necessary for the actual computation of radiative transfer can be represented by the Henyey–Greenstein phase function involving the asymmetry factor alone as a parameter:

$$P(\mu, \mu') = \sum_{n=0}^{\infty} (2n+1) \tilde{g}^n P_n(\mu) P_n(\mu') = \frac{2(1-\tilde{g}^2)}{\pi} \frac{E(k^2)}{(A'-B')\sqrt{A'+B'}} \quad (6.35)$$

$$\left. \begin{aligned} A' &= 1 + \tilde{g}^2 - 2\tilde{g}\mu\mu' \\ B' &= 2|\tilde{g}|\sqrt{1-\mu^2}\sqrt{1-\mu'^2} \\ k^2 &= 2B'/(A'+B') \end{aligned} \right\} \quad (6.36)$$

Here, $E(k^2)$ represents the complete elliptic integral of the second kind. Moreover, $\tilde{g}$ should be read as $\tilde{g}^*$ when the scaled scattering phase function is required. In computing β or β^* from Eqs. (6.29) or (6.32), D_c plays a vital role and thus guidelines for D_c are required: the measured pore diameter D_m should be used as D_c whenever its information is available, otherwise D_c should be estimated from $(1-w)D_n$. Here, D_n represents the nominal cell diameter defined by $2.54 \times 10^{-2}/\text{PPI}$ (m) and PPI denotes the manufacturer-provided mean pores per inch value. As seen from Figure 6.5, the experimental data for β and β^* are well correlated with our formulas: Eqs. (6.29) or (6.32) approximate 94% of the data with an accuracy of less than $\pm 25\%$. Comparisons of theoretical predictions for ω_λ and $\tilde{g}_\lambda$ with corresponding experimental data are shown in Figures 6.6 and 6.7. The experimental data were taken from the report of Hendricks and Howell [24] and the spectral reflectivity of the solid needed for computations of ω_λ and $\tilde{g}_\lambda$ were taken from Touloukian's data compilation [25]. The agreement between theory and experiment seems to be reasonable because a value of ρ_H appreciably depends on the surface condition of the material such as the roughness and composition, which may vary from sample to sample.

6.3.4

Fluid Mechanical Properties

The momentum Eq. (6.2) involves two empirical parameters K and F that must be determined experimentally. In the case of packed-sphere systems, the following

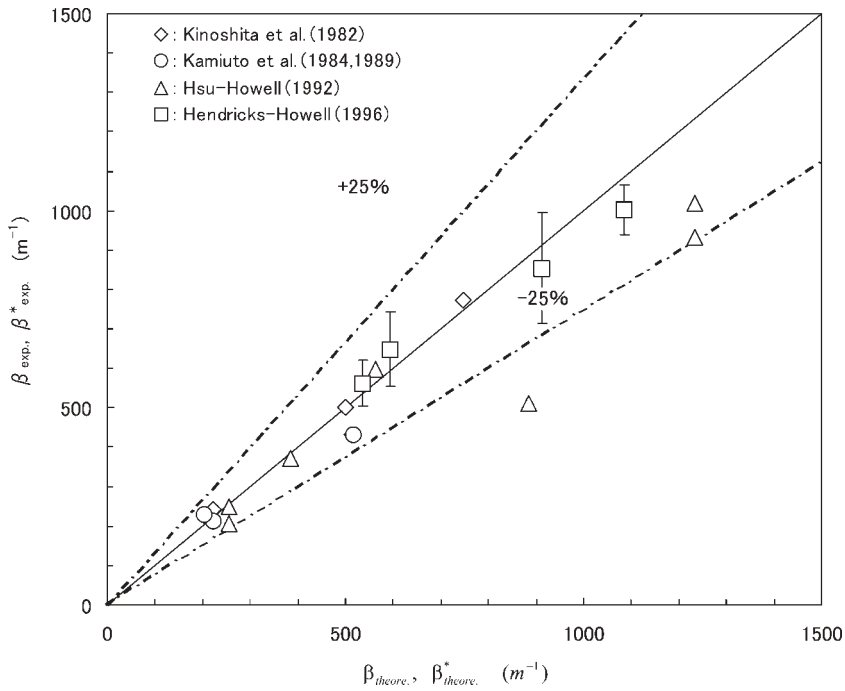


Figure 6.5 Correlation between theoretical values of β and β^* predicted from Kamiuto's model and available experimental values of β and β^* .

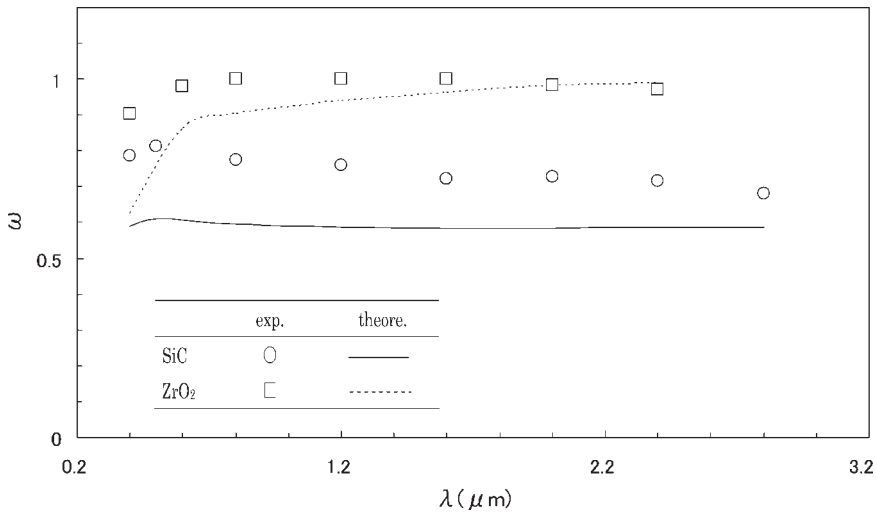


Figure 6.6 Spectral variations in the albedos of oxide-bonded SiC and partially stabilized ZrO₂ porous materials.

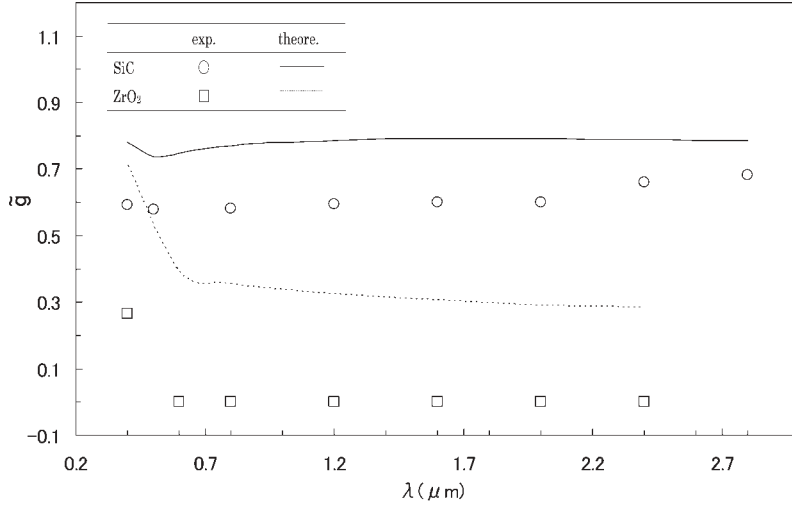


Figure 6.7 Spectral variations in the asymmetry factors of oxide-bonded SiC and partially stabilized ZrO₂ porous materials.

correlations derived by Ergun [26] have been widely used:

$$\left. \begin{aligned} K &= d_p^2 \phi^3 / 150(1-\phi)^2 \\ F &= \left(1.75 / \sqrt{150} \right) / \phi^{1.5} \end{aligned} \right\} \quad (6.37)$$

where d_p represents mean sphere diameter. As for open-cell foams, Du Plessis *et al.* [27] and Bhattacharya *et al.* [14] presented semi-empirical expressions for evaluating K and F , but the validity of the proposed formulas was tested using their own data alone.

Here, we propose empirical formulas involving two parameters, i.e. porosity ϕ and an equivalent strut diameter as a cylinder, D_p :

$$\left. \begin{aligned} K &= a_1 \phi^{a_2} D_p^{a_3} \\ F &= b_1 (1-\phi)^{b_2} \\ D_p &= 2D_n w / \sqrt{\pi} \end{aligned} \right\} \quad (6.38)$$

Values of the parameters involved in K and F were determined using a least-squares method by applying these expressions to available experimental data including those obtained by our group in Oita:

$$\left. \begin{aligned} a_1 &= 3.824, & a_2 &= 24.93, & a_3 &= 1.947 \\ b_1 &= 0.714, & b_2 &= 0.673 \end{aligned} \right\} \quad (6.39)$$

Correlations between predictions based on Eqs. (6.38) and experimental data are shown in Figures 6.8 and 6.9. In these figures, the data obtained by Bhattacharya *et al.* were disregarded because their results for F depict a rather peculiar trend: values of F are almost constant against ϕ . As seen from Figures 6.8 and 6.9,

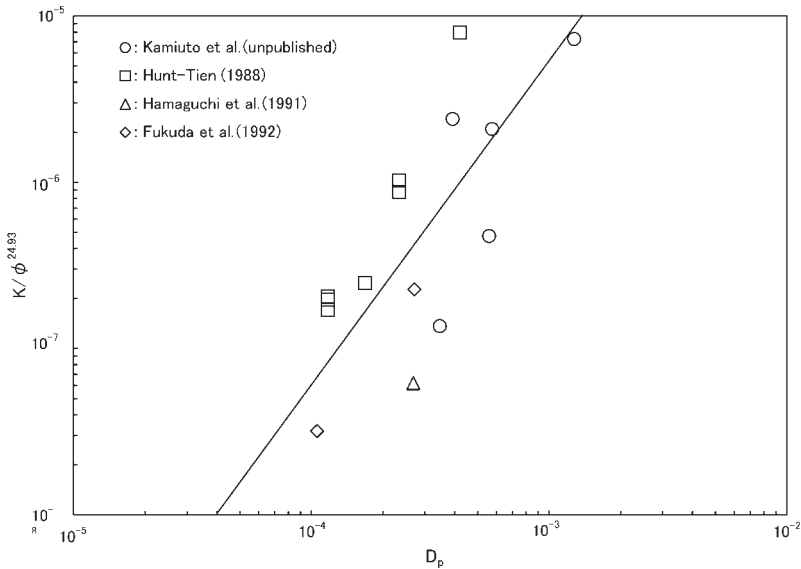


Figure 6.8 Permeability K as a function of equivalent strut diameter D_p : experiment versus least-squares fit.

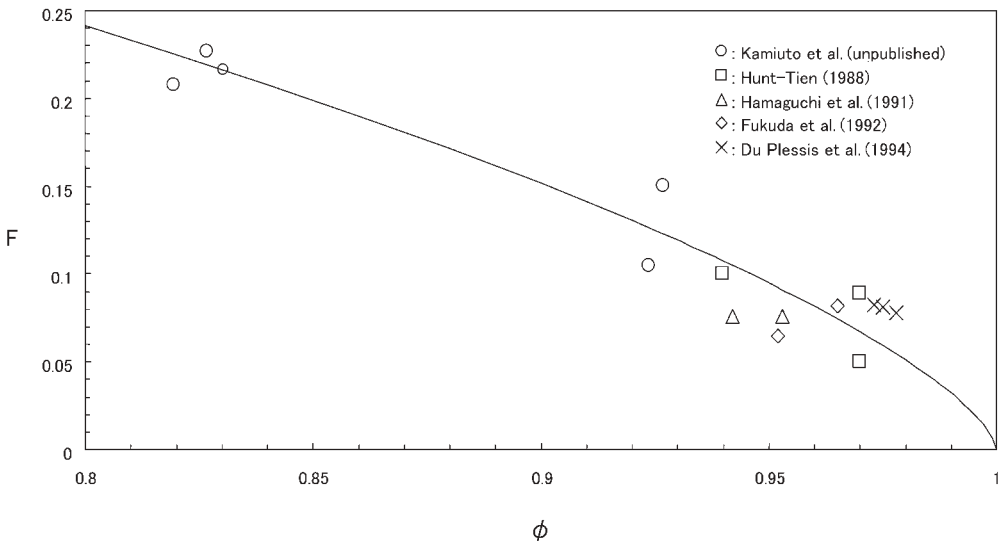


Figure 6.9 Inertial coefficient F as a function of porosity: experiment versus least-squares fit.

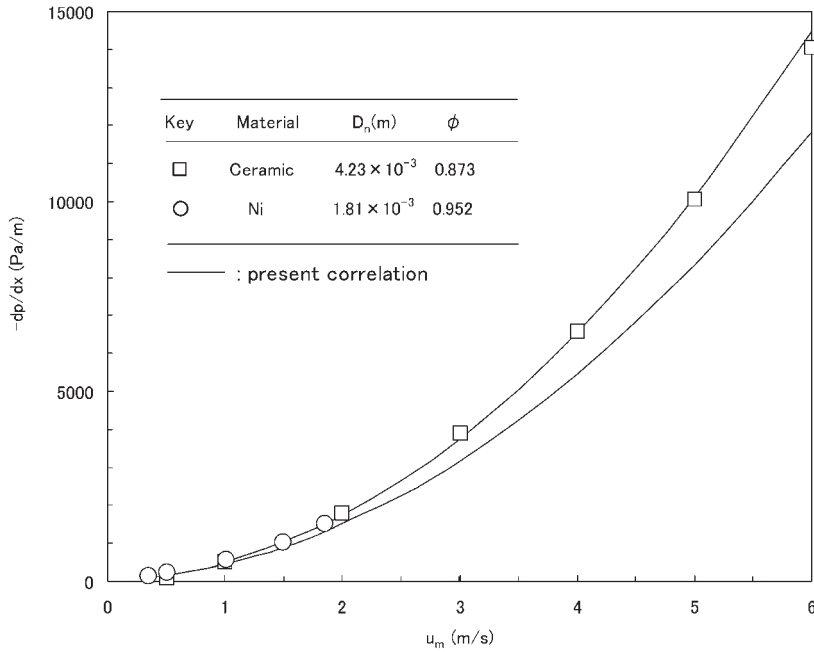


Figure 6.10 Relations between pressure gradient in the flow direction and mean flow velocity.

Eqs. (6.38) and (6.39) reasonably correlate with the experimental data. For a slug flow in a porous duct, the pressure drop can be estimated from

$$-\frac{dP}{dx} = \frac{\mu_f}{K} u_m + \frac{\rho_f F}{\sqrt{K}} u_m^2 \quad (6.40)$$

The validity of this pressure drop equation together with Eqs. (6.38) and (6.39) is shown in Figure 6.10.

6.3.5

Volumetric Heat Transfer Coefficient

The volumetric heat transfer coefficient between the fluid and solid phases, h_v , appearing in Eqs. (6.3) and (6.4) has been determined using transient response techniques. In almost all the previous studies, however, the axial diffusion terms in the energy equation for the fluid phase have been omitted, and thus the results obtained for h_v contain effects of the axial thermal dispersion and/or fluid conduction. Generally, heat transfer data are represented in form of Nusselt number as defined by

$$Nu_i = h_v l_i^2 / k_f \quad (6.41)$$

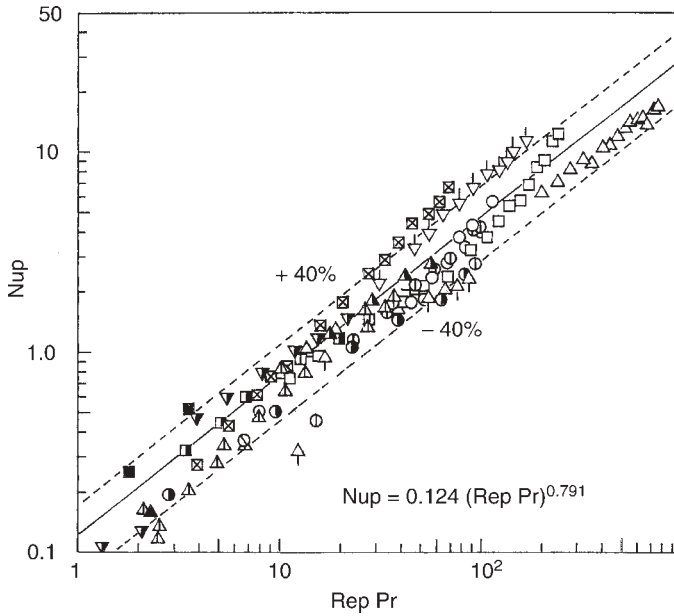


Figure 6.11 Relations between the Nusselt number Nu_p and the Peclet number $Re_p Pr$.

Here, l_i represents an appropriate characteristic length of an examined porous medium.

Younis and Viskanta [28] used actual pore diameter as l_i , while Hamaguchi *et al.* [29] adopted measured strut diameter. Fukuda *et al.* [30] recommended using $\sqrt{K}$ as l_i . Kamiuto and Yee [31] examined various characteristic lengths to obtain a better correlation for the heat transfer coefficient and recommended adopting an equivalent strut diameter D_p defined by Eq. (6.38). Based on this characteristics length, available experimental data for h_v can be correlated by

$$Nu_p = h_v D_p^2 / k_f = 0.124 (Re_p Pr)^{0.791} \quad (6.42)$$

They reported that Eq. (6.42) reproduces 78.1% of available experimental data with an error less than $\pm 40\%$ as shown in Figure 6.11.

6.4 Radiative Transfer

In order to test the validity of the radiative property model and transfer-theoretical approach summarized in Section 6.3.3, spectral or total normal emittances of isothermal, plane-parallel, open-cellular porous plates are evaluated theoretically by

solving the equation of transfer and the results obtained are compared with available experimental data. Obviously, predictions of emission characteristics of an open-cell foam are of practical importance in connection with thermal design of high-temperature equipments such as porous radiant burners and radiant porous fins. To perform numerical analyses [32], the following assumptions are introduced: (a) a plane-parallel, open-cellular porous plate of thickness y_0 is installed horizontally and is bounded by both an upper vacuum boundary and a lower opaque diffuse solid one; (b) the porous plate and the solid boundary are isothermal and are kept at a temperature T_m (K); (c) the vacuum boundary is uniformly irradiated by blackbody radiation characterized by an environmental temperature T_∞ (K); (d) the porous plate is quasi-homogeneous and is capable of emitting, absorbing and anisotropically scattering thermal radiation; (e) the scattering phase function can be represented by Henyey–Greenstein's phase function and is governed by the asymmetry factor $\bar{g}$ alone; (f) the radiative properties of an open-cell foam are described by Kamiuto's model; (g) the scaled extinction coefficient and the scaled asymmetry factor of the scattering phase function are gray and do not depend on temperature; and (h) the hemispherical reflectivity of surface of the struts and strut junctures of an open-cell foam is treated to be nongray or gray, depending on available reflectivity data.

Under these assumptions, the equation of transfer and associated boundary conditions may be written as follows. For a nongray case

$$\begin{aligned} \mu \frac{\partial I_\lambda(y, \mu)}{\partial y} + \beta^* I_\lambda(y, \mu) &= \beta^* (1 - \omega_\lambda^*) I_{b\lambda}(T_m) \\ &+ \frac{\beta^* \omega_\lambda^*}{2} \int_{-1}^1 P^*(\mu, \mu') I_\lambda(y, \mu') d\mu' \end{aligned} \quad (6.43)$$

The boundary conditions to Eq. (6.43) are

$$\left. \begin{aligned} y = 0 : \quad I_\lambda(0, \mu > 0) &= I_{b\lambda}(T_m) \\ y = y_0 : \quad I_\lambda(y_0, \mu < 0) &= \varepsilon_w I_{b\lambda}(T_m) + 2(1 - \varepsilon_w) \int_0^1 I_\lambda(y_0, \mu') \mu' d\mu' \end{aligned} \right\} \quad (6.44)$$

For a gray case

$$\mu \frac{\partial I(y, \mu)}{\partial y} + \beta^* I(y, \mu) = \beta^* (1 - \omega^*) \frac{\sigma T_m^4}{\pi} + \frac{\beta^* \omega^*}{2} \int_{-1}^1 P^*(\mu, \mu') I(y, \mu') d\mu' \quad (6.45)$$

Its associated boundary conditions are

$$\left. \begin{aligned} y = 0 : \quad I(0, \mu > 0) &= \frac{\sigma T_\infty^4}{\pi} \\ y = y_0 : \quad I(y_0, \mu < 0) &= \varepsilon_w \frac{\sigma T_m^4}{\pi} + 2(1 - \varepsilon_w) \int_0^1 I(y_0, \mu') \mu' d\mu' \end{aligned} \right\} \quad (6.46)$$

Table 6.1 Physical characteristics of the examined open-cellular porous materials.

Material	Porosity, ϕ	PPI	Thickness (mm)	Ref.
Al_2O_3 (80 wt%)- SiO_2 (20 wt%)	0.85	30.5	154	[38]
Nickel (70 wt%)-chromium (30 wt%)	0.937	8.5	10.3	[36]
Cordierite ($2\text{MgO} \cdot 2\text{Al}_2\text{O}_3 \cdot 5\text{SiO}_2$)	0.873	6	11.9	[36]

The equation of transfer, Eqs. (6.43) and (6.45), together with their relevant boundary conditions are solved using Barkstrom's finite difference method [33]. Once the equation of transfer is solved numerically and the radiation field is specified, the spectral or total normal emittances may be readily evaluated as follows:

$$\left. \begin{aligned} \varepsilon_{N,\lambda} &= I_\lambda(0, -1)/I_{b\lambda}(T_m) \\ \varepsilon_N &= I(0, -1)/(\sigma T_m^4/\pi) \end{aligned} \right\} \quad (6.47)$$

Three kinds of open-cellular porous material are considered to test the validity of Kamiuto's model: Al_2O_3 (80 wt%)- SiO_2 (20 wt%), Ni (70 wt%)-Cr (30 wt%) and cordierite ($2\text{MgO} \cdot 2\text{Al}_2\text{O}_3 \cdot 5\text{SiO}_2$) foams. The physical characteristics of the examined open-cellular porous materials are summarized in Table 6.1. Spectral data of the normal reflectivity of Al_2O_3 - SiO_2 solid were taken from Ref. [34], but, to take into account the uncertainty of the surface conditions of the tested material, values of spectral reflectivity were increased by 15% of the original data in accord with Fu *et al.* [35]. Experimental data of the total hemispherical reflectivity of Ni-Cr and cordierite foams were taken from Ref. [36] and are represented by the following expressions:

$$\left. \begin{aligned} \rho_H &= 0.698 + 0.26\delta \quad \text{for cordierite} \\ \rho_H &= -1.51 + \delta(14.22 + \delta\{-40.54 + \delta[54.82 + \delta(-35.5 + 8.81\delta)]\}) \\ &\quad \text{for Ni-Cr} \end{aligned} \right\} \quad (6.48)$$

Here, δ is defined by $T/1000$ (K).

The hemispherical emissivity of the bottom surface of an Al_2O_3 - SiO_2 foam was assumed to be unity, whereas that of Ni-Cr and cordierite foam, i.e. the hemispherical emissivity of oxidized SUS 304 plate, was represented by the following expression [37]:

$$\varepsilon_w = 0.326 + 0.295\delta \quad (6.49)$$

Figure 6.12 shows measured and predicted spectral variations in the normal emittance of the Al_2O_3 - SiO_2 open-cell foam. Measured data were obtained by

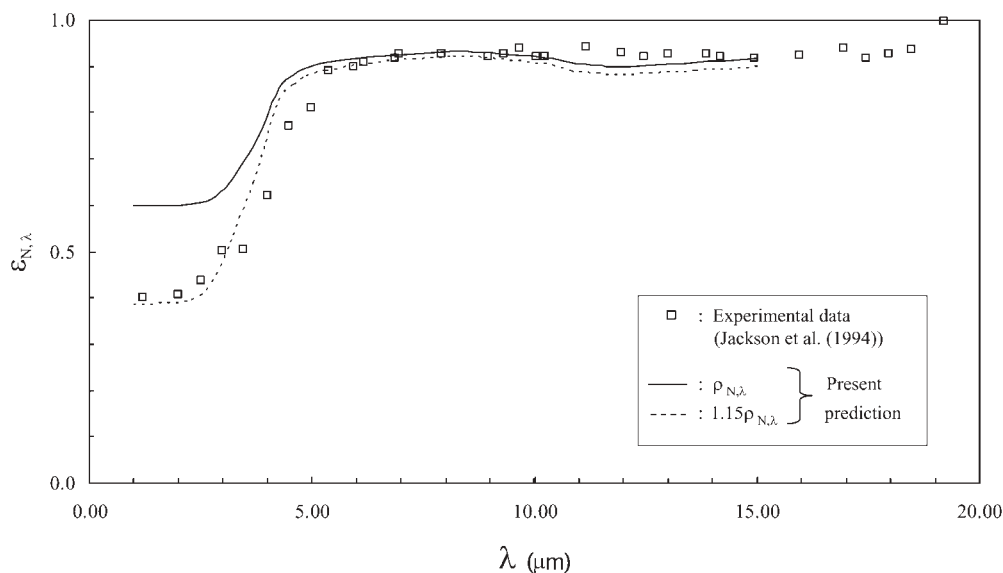


Figure 6.12 Predicted and measured spectral variations in the normal emittance of an $\text{Al}_2\text{O}_3\text{--SiO}_2$ open-cell foam.

Jackson *et al.* [38]. The spectral normal emittance increase from about 0.4 to 0.9 as the wavelength increases from 1 to $6\mu\text{m}$: this exactly corresponds to the spectral variations in the normal emissivity of alumina–silicate solid given by $1 - \rho_{N,\lambda}$. As seen from Figure 6.12, the predicted emittance agrees well with the experimental results for $\lambda > 6\mu\text{m}$. However, for $\lambda < 6\mu\text{m}$, the predicted results are higher than the experimental ones. Obviously, this is caused by the fact that $\rho_{N,\lambda}$ depends on the surface conditions of the material, which seems to change from sample to sample. To take into account this uncertainty, the predictions based on $1.15\rho_{N,\lambda}$ were also made, which shows much closer agreement with the experimental data. Figure 6.13 depicts the variation of the total normal emittances of Ni–Cr and cordierite foams against mean foam temperature. In accord with temperature variations of the total hemispherical emissivity, i.e. $1 - \rho_{N,\lambda}$, the total normal emittance decreases with an increase in foam temperature. There exist some discrepancies between theory and experiment, particularly for the cordierite foam in a temperature region less than about 500–600 K due to the low sensitivity of a radiation detector (thermopile) used in the experiment; in a temperature region greater than 500–600 K, satisfactory agreement is achieved.

Thus it may be concluded that the spectral or total emission characteristics of an isothermal open-cellular porous plate can be accurately predicted by a transfer-theoretical approach based on Kamiuto's radiative property model.

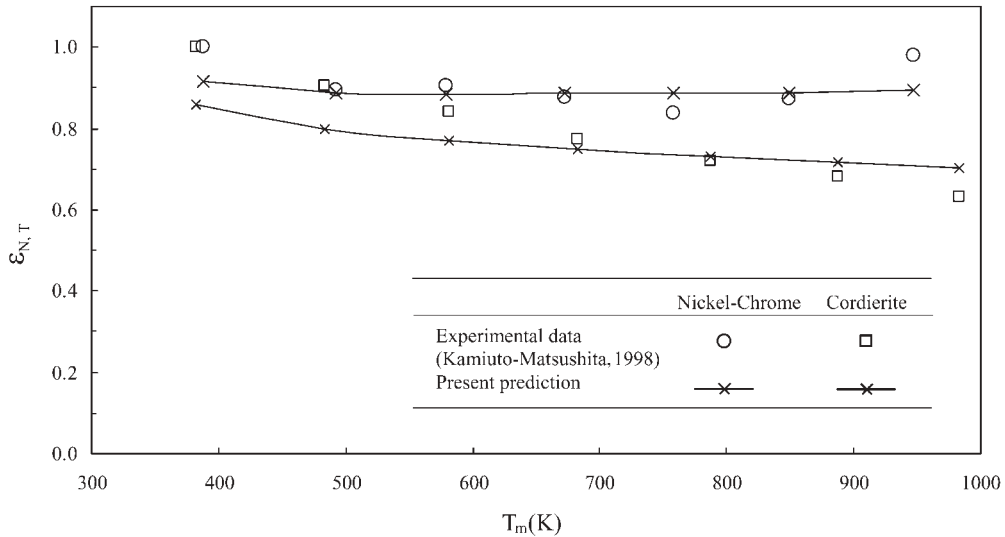


Figure 6.13 Variations of predicted and measured total normal emittances of Ni-Cr and cordierite foams against mean foam temperature.

6.5 Combined Conductive and Radiative Heat Transfer

Coupled conduction and radiation heat transfer in open-cellular porous media has been studied by many researchers in connection with thermal design of open-cell foam insulation at high temperatures. The aim of this section is to discuss the ability of the aforementioned theoretical models for elementary transport processes in open-cellular porous media in predicting temperature profiles and mean total effective thermal conductivities in porous media, and thus only a few relevant previous studies are referred to here.

Kinoshita *et al.* [39] and Kamiuto *et al.* [40] made fundamental studies of combined conductive and radiative heat transfer in cordierite and Ni-Cr porous plates. On the basis of the radiative properties determined experimentally by their own inverse scattering problem resolvers and available empirical formulas for the effective thermal conductivity by conduction alone, they could accurately predict temperature profiles and heat transfer characteristics of the porous plates. Glicksman *et al.* [41] fully examined elementary thermal processes in polyurethane foam insulation and found that the conduction process can be described using simple parallel-series models. In addition, they determined the absorption and scattering coefficients and phase function experimentally. These previous studies, however, are more or less empirical because experimentally determined thermophysical properties were incorporated into the analyses. In what follows, we perform purely theoretical analyses [42]. The following assumptions are introduced for this purpose: (a) a plane-parallel,

open-cellular porous plate is installed horizontally and bounded by two opaque diffuse solid plates; (b) the porous plate is heated from above and cooled from below; (c) heat transfer across the plate is due to conduction and radiation; (d) the porous plate is capable of emitting, absorbing and anisotropically scattering thermal radiation; (e) all the radiative properties are gray; and (f) relevant physical properties depend on temperature.

Under these assumptions, the energy equation may be written as follows:

$$\frac{d}{dy} \left[k_{\text{eff},c} \frac{dT}{dy} \right] = \beta^* (1 - \omega^*) (4\sigma T^4 - G) \quad (6.50)$$

The boundary conditions for Eq. (6.50) are

$$\left. \begin{aligned} y = 0 : \quad T &= T_H \\ y = y_0 : \quad T &= T_L (< T_H) \end{aligned} \right\} \quad (6.51)$$

In Eq. (6.50), G represents the incident radiation and is defined by $2\pi \int_{-1}^1 I(y, \mu) d\mu$.

The intensity of radiation $I(y, \mu)$ is governed by

$$\mu \frac{\partial I(y, \mu)}{\partial y} + \beta^* I(y, \mu) = \beta^* (1 - \omega^*) \frac{\sigma T^4}{\pi} + \frac{\omega^* \beta^*}{2} \int_{-1}^1 P^*(\mu, \mu') I(y, \mu') d\mu' \quad (6.52)$$

where $P^*(\mu, \mu')$ is given by the Henyey–Greenstein phase function with the scaled asymmetry factor $\bar{g}^*$. The boundary conditions for Eq. (6.52) are given by Eq. (6.11). The P_1 approximation explained in Section 6.2 was also utilized.

The energy equation and the equation of transfer (or the P_1 equations) were solved numerically using finite difference schemes. Once both the temperature and radiation fields are determined, we can readily evaluate the heat transfer characteristics. The total heat flux q_t is computed from

$$q_t = q_C + q_R \quad (6.53)$$

$$q_C = -k_{\text{eff},c}(T) \frac{dT}{dy} \quad (6.54)$$

$$q_R = 2\pi \int_{-1}^1 I(y, \mu') \mu' d\mu' \quad (6.55)$$

The mean total effective thermal conductivity $\bar{k}_{\text{eff},t}$ is defined as follows:

$$\bar{k}_{\text{eff},t} = q_t y_0 / (T_H - T_L) \quad (6.56)$$

The physical properties needed for the analyses are the effective thermal conductivity by conduction alone $k_{\text{eff},c}$ and radiative properties: these were estimated using Dul'nev's formula, Eq. (6.17), and our radiative property model. To examine the validity of the present theoretical approach, the numerical computations were made under conditions corresponding to the experiments for cordierite and zirconia porous plates reported previously [21,39,40].

The hemispherical reflectivities and thermal conductivities of cordierite and zirconia were taken from the literature:

$$\left. \begin{aligned} \rho_H &= 0.698 + 0.26\delta \text{ for cordierite} \\ \rho_H &= 0.475 - 1.926\delta + 5.107\delta^2 - 4.634\delta^3 + 1.826\delta^4 - 0.27\delta^5 \text{ for zirconia} \end{aligned} \right\} \quad (6.57)$$

$$\left. \begin{aligned} k_s(\text{Wm}^{-1}\text{K}^{-1}) &= 2.29 - 0.21\delta \text{ for cordierite} \\ k_s(\text{Wm}^{-1}\text{K}^{-1}) &= (73.03 + 404.98\delta - 1999.89\delta^2 + 2241.52\delta^3) / \\ &\quad (1 + 376.62\delta - 1332.16\delta^2 + 1351.6\delta^3) \text{ for zirconia} \end{aligned} \right\} \quad (6.58)$$

The results obtained are depicted in Figures 6.14 to 6.16. Figure 6.14 shows temperature profiles in a 0.05 m thick cordierite porous plate ($\phi = 0.873$ and $D_c = 0.00324$ m) bounded by a SUS304 plate (we assumed that $\epsilon_L = 0.5$) used as the cold boundary and a SUS310S plate ($\epsilon_H = 0.032 + 0.39(T_H/1000)$) used as the hot boundary. The temperature profiles deviate from a linear distribution and come to have a steep gradient at the cold boundary as the hot boundary temperature is raised, because the porous medium near the cold boundary is heated appreciably by heat radiation from the hot boundary and by self-emission due to the heated porous medium. Figures 6.15 and 6.16 show variations in the mean total effective thermal conductivity $\bar{k}_{\text{eff},t}$ against the mean layer temperature. $\bar{k}_{\text{eff},t}$ increases with the mean layer temperature and decreases with an increase in the mean cell

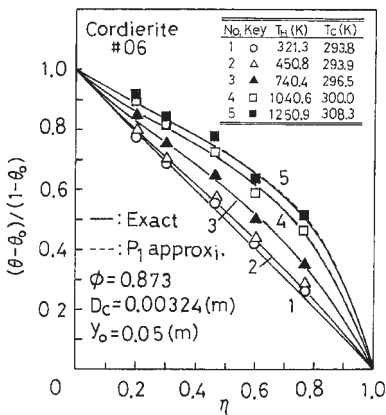


Figure 6.14 Temperature profiles in a 0.05 m thick cordierite porous plate with $\phi = 0.873$ and $D_c = 0.00324$ m.

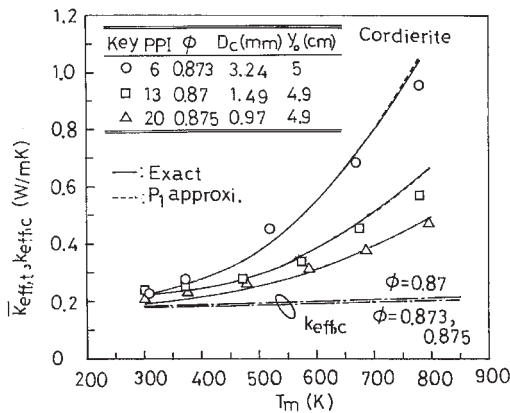


Figure 6.15 Relations between the mean total effective thermal conductivity of cordierite porous plate and mean plate temperature.

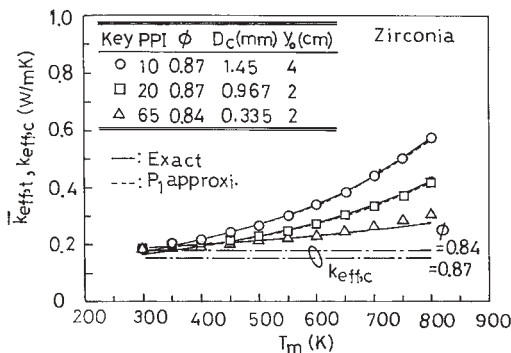


Figure 6.16 Relations between the mean total effective thermal conductivity of zirconia porous plate and mean plate temperature.

diameter, provided that other parameters remain unchanged. It is found that theoretical results based on the exact analysis agree well with the experimental ones and, moreover, there is only a small difference between the exact numerical analysis and the approximate one based on the P_1 approximation.

6.6

Combined Forced-Convective and Radiative Heat Transfer

Paying attention to the high volumetric heat transfer coefficients and large radiation extinction coefficients of open-cellular porous materials, several thermal engineering researchers have proposed heat transfer equipments using open-cell foams: porous radiation shields [43,44], porous extended surfaces [45], porous radiant burners [46–48], porous gas enthalpy-radiation converters [2], and so on.

In this section, we refer to two typical applications of open-cell foams, i.e. a gas enthalpy-radiation conversion system and transpiration cooling system.

6.6.1

Analysis of Gas Enthalpy-Radiation Conversion System

To recover as much as possible of the enthalpy of exhaust gases from various furnaces, Echigo [2] presented an idea of placing porous materials vertically to the flow direction in an exhaust duct and proved a remarkable effect experimentally: the temperature falls of an exhaust gas reach 100–200 K while passing through a foam metal of 15 mm thickness. Echigo [2] also made a theoretical analysis of this system, but he disregarded the effect of scattering, which was later taken into account by Wang and Tien [49]. In what follows, we present a predictive model for gas enthalpy-radiation conversion processes in an open-cellular porous plate. The proposed model is based on the following assumptions: (a) the flow field is one-dimensional; (b) the working fluid is a nonradiating gas; (c) an open-cellular porous plate is placed normal to the flow direction in a straight duct; (d) the porous plate can absorb, emit and anisotropically scatter thermal radiation; (e) the radiative properties of the porous plate are described by Kamiuto's model in Section 3.3 and do not depend on the wavelength; and (f) all the physical properties depend on temperature.

Under these assumptions, the law of conservation of energy for each phase yields the following expressions:

$$\rho_f C_{Pf} u \frac{dT_f}{dy} = -h_v(T_f - T_s) + \phi \frac{d}{dy} \left[k_f \frac{dT_f}{dy} \right] \quad (6.59)$$

$$f(1-\phi) \frac{d}{dx} \left[k_s \frac{dT_s}{dy} \right] + h_v(T_f - T_s) - \text{div} \mathbf{q}_R = 0 \quad (6.60)$$

$$\text{div} \mathbf{q}_R = \beta^* (1-\omega^*) (4\sigma T^4 - G) \quad (6.61)$$

The boundary conditions to Eqs. (6.59) and (6.60) are

$$\left. \begin{aligned} y = 0 : \quad T_f &= T_0, \quad \frac{dT_s}{dy} = 0 \\ y = y_0 : \quad \frac{dT_f}{dx} &= \frac{dT_s}{dy} = 0 \end{aligned} \right\} \quad (6.62)$$

The P_1 equations for G and q_R are

$$\left. \begin{aligned} \frac{dG}{dy} + 3\beta^* (1-\omega^* \bar{g}^*) q_R &= 0 \\ \frac{dq_R}{dy} + \beta^* (1-\omega^*) G &= 4\beta^* (1-\omega^*) \sigma T^4 \end{aligned} \right\} \quad (6.63)$$

The Marshak boundary conditions for Eq. (6.63) are

$$\left. \begin{array}{l} \gamma = 0 : \quad G + 2q_R = 4\sigma T_{bu}^4 \\ \gamma = \gamma_0 : \quad G - 2q_R = 4\sigma T_{bd}^4 \end{array} \right\} \quad (6.64)$$

Here, T_{bu} and T_{bd} , respectively, represent the equivalent blackbody temperatures of radiation incoming from the upstream and downstream regions. The energy equations were solved using an implicit finite difference method, while P_1 equations were solved using our staggered scheme [50].

To examine the ability of the proposed model in predicting temperature profiles within a porous converter, computations were made under conditions corresponding to the experiments by Echigo [2]. Here, we assumed that $T_{bd} = T_\infty = 300$ [K] and $T_{bu} = 850$ [K]. Results are shown in Figure 6.17, where the dimensionless quantities are defined by $\theta_f = T_f/T_\infty$ and $\theta_s = T_s/T_\infty$. Agreement between the experimental data obtained by Echigo and our predictions is quite satisfactory, and this confirms the validity of the proposed theoretical model.

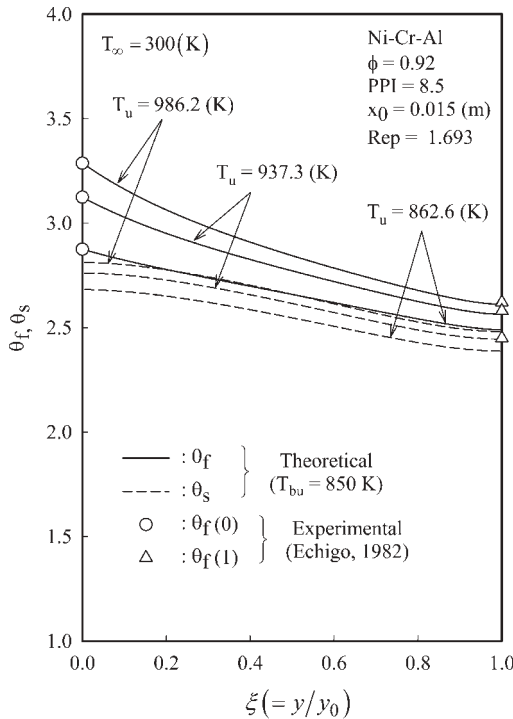


Figure 6.17 Temperature profiles within a 15 mm thick Ni–Cr–Al porous plate.

6.6.2

Analysis of Transpiration Cooling System in a Radiative Environment

Transpiration cooling is a well-known technique for protecting a structure from a high-temperature environment such as a large fire involving a hydrocarbon pool or storage. In this thermal shield system, high-intensity irradiation from the environment is absorbed and scattered by porous media made of open-cell foams or sintered metals and a major part of the radiant energy absorbed by the porous media is converted into heat, which is transferred to gas flowing through the porous media or reemitted. In this section, we perform an analysis of combined convective and radiative heat transfer in a transpiration cooling system using open-cellular porous materials subject to irradiation from the environment and compare results obtained with available experimental data [44]. The physical model and coordinate systems are shown in Figure 6.18. To perform the theoretical analysis, the following assumptions are introduced: (a) the heat shield consists of a one-dimensional layer of open-cellular porous material; (b) the front surface of the heat shield is uniformly irradiated by blackbody radiation characterized by an equivalent temperature T_R (K), while the back surface is subject to uniform blackbody radiation characterized by an inlet air temperature T_0 (K); (c) low-temperature air is injected through the back surface of the heat shield; (d) air is transparent to thermal radiation; (e) the heat shield is able to absorb, emit and scatter thermal radiation, but its radiative properties do not depend on wavelength and temperature; (f) the relevant physical properties do not depend on temperature; (g) both solid and gas phases can be regarded as continuous ones; and (h) heat transfer with the heat shield is in a steady state.

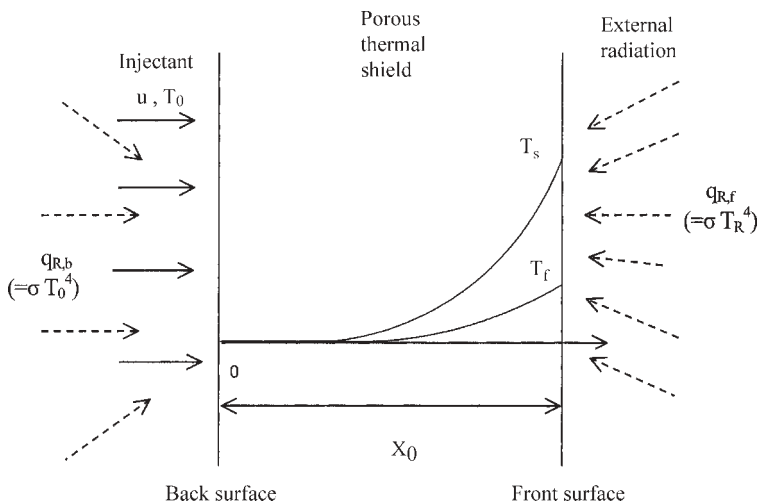


Figure 6.18 Physical model and coordinate systems of transpiration cooling system using open-cellular porous materials.

Under these assumptions, the governing energy equations for the gas and solid may be written as

$$\rho_f C_{pf} u \frac{dT_f}{dx} = \phi k_f \frac{d^2 T_f}{dx^2} - h_v (T_f - T_s) \quad (6.65)$$

$$\frac{1}{3} (1-\phi) k_s \frac{d^2 T_s}{dx^2} + h_v (T_f - T_s) - \text{div} \mathbf{q}_R = 0 \quad (6.66)$$

$$\text{div} \mathbf{q}_R = \beta^* (1-\omega^*) (4\sigma T_s^4 - G) \quad (6.67)$$

where T_f and T_s , respectively, denote the temperatures of the fluid and solid phases. G represents the incident radiation and is determined by solving the following P_1 equation:

$$\frac{d^2 G}{dx^2} - 3\beta^* (1-\omega^*) (1-\omega^* \bar{g}^*) G = -12\beta^* (1-\omega^*) (1-\omega^* \bar{g}^*) \sigma T_s^4 \quad (6.68)$$

The boundary conditions for Eqs. (6.65), (6.66) and (6.68) are given as follows:

$$\left. \begin{aligned} x=0: \quad T_f &= T_0, \quad \frac{dT_s}{dx} = 0, \quad G(0) - \frac{2}{3\beta^* (1-\omega^* \bar{g}^*)} \frac{dG}{dx} \Big|_{x=0} = 4\sigma T_0^4 \\ x=x_0: \quad \frac{dT_f}{dx} &= \frac{dT_s}{dx} = 0, \quad G(x_0) + \frac{2}{3\beta^* (1-\omega^* \bar{g}^*)} \frac{dG}{dx} \Big|_{x=x_0} = 4\sigma T_R^4 \end{aligned} \right\} \quad (6.69)$$

The governing equations are rewritten in dimensionless form and then are solved numerically using a finite difference method. After obtaining distributions for T_f , T_s and G , three kinds of figure of merit are evaluated:

$$\eta_T = (T_R - (T_s(0) + T_s(x_0))/2) / (T_R - T_0) \quad (6.70)$$

$$\eta_C = \rho_f C_{pf} u (T_f(x_0) - T_f(0)) / q_{R,f} \quad (6.71)$$

$$\eta_R = 2\pi \int_0^1 I(x_0, \mu) \mu d\mu / q_{R,f} \quad (6.72)$$

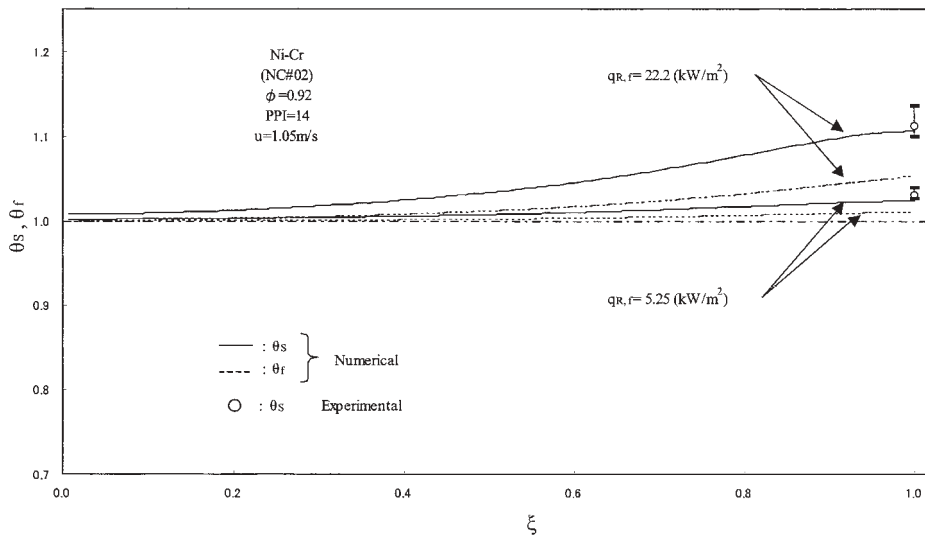
where $q_{R,f}$ denotes the radiative heat flux from an environmental radiation source. In the expressions, η_T indicates a temperature efficiency, which is an index representing how close the mean temperature of the heat shield is to the inlet air temperature, η_C denotes a ratio of fluid enthalpy rise to the incoming radiant energy and η_R represents the slab reflectance, i.e. a ratio of the radiant energy directed toward the environment from the heat shield to the incoming radiant energy. Here, it should be noted that the radiant energy directed towards the environment from the heat shield

Table 6.2 Physical characteristics of the examined porous media.

Material	Thickness, x_0 (m)	Porosity, ϕ	Pores per inch, PPI	Extinction coefficient, β^* (m^{-1})
Nickel–chromium (NC#02)	0.01	0.92	14	1.94×10^2
Cordierite–alumina (CA#06)	0.012	0.89	6	1.02×10^2

involves the amount of radiant energy emitted from the porous medium itself and originating from the region upstream.

Two kinds of open-cellular porous material are used: cordierite-Alumina ($\text{Al}_2\text{O}_3/54$ wt%, $\text{SiO}_2/37$ wt%, $\text{MgO}/6$ wt% and the others/3 wt%) and Ni–Cr (Ni/80 wt% and Cr/20 wt%). The physical characteristics of the examined porous media are summarized in Table 6.2. Moreover, the physical properties of the examined porous media are described in Section 6.4. Typical temperature profiles of the solid and gas phases inside the Ni–Cr porous heat shield are shown in Figure 6.19, where ξ is defined by x/x_0 . The measured mean surface temperatures of the porous heat shield are indicated by open circles, while the calculated results for $\theta_s (=T_s/T_0)$ and $\theta_f (=T_f/T_0)$ are, respectively, represented by solid and broken lines. The temperatures of both phases increase with irradiation near the exit region: this is the case irrespective of the kinds of porous medium. Figures 6.20 and 6.21 illustrate variations in the temperature efficiency η_T against $Re_p (=uD_p/\nu_f)$. The experimental results are shown by symbols, while the numerical results are indicated by solid lines.

**Figure 6.19** Temperature profiles within a Ni–Cr open-cellular porous heat shield.

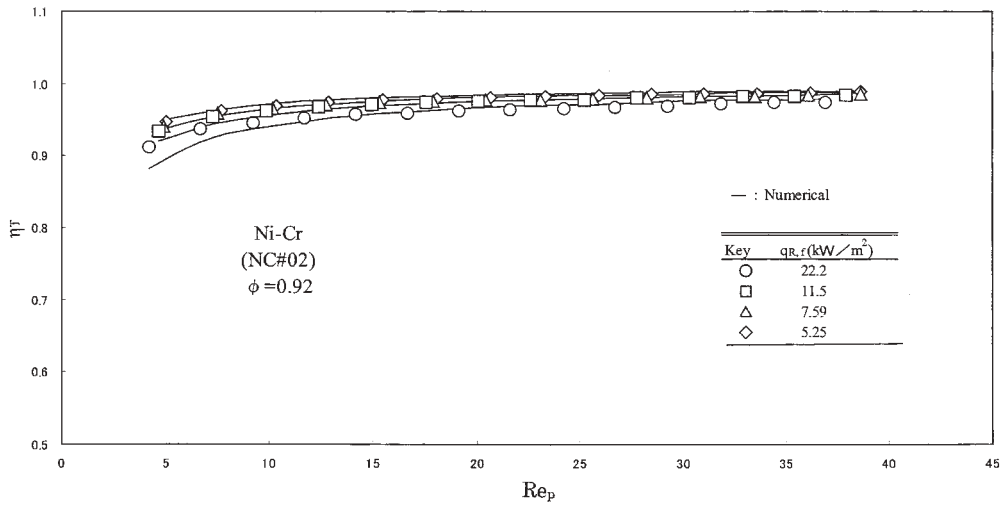


Figure 6.20 Variations in the temperature efficiency of a Ni-Cr open-cellular porous heat shield against the Reynolds number Re_p .

η_T increases with Re_p and is asymptotic to constant values, depending on a level of the incident radiation. Values of η_T are greater than 0.9 for $Re_p \geq 10$, irrespective of the kinds of porous material, meaning that the average heat shield temperature is very close to the inlet air temperature. Agreement between theory and experiment is acceptable, and this substantiates the validity of the present theoretical model. To

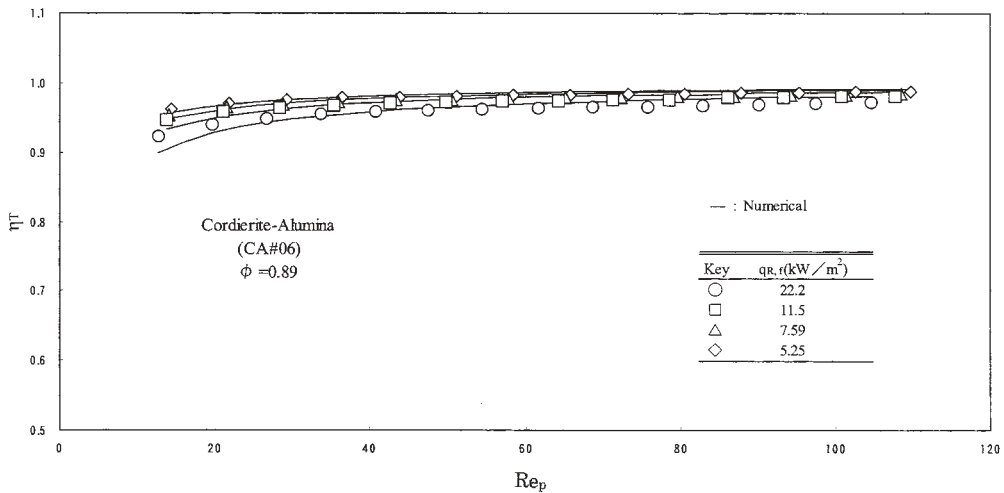


Figure 6.21 Variations in the temperature efficiency of a cordierite-alumina open-cellular porous heat shield against the Reynolds number Re_p .

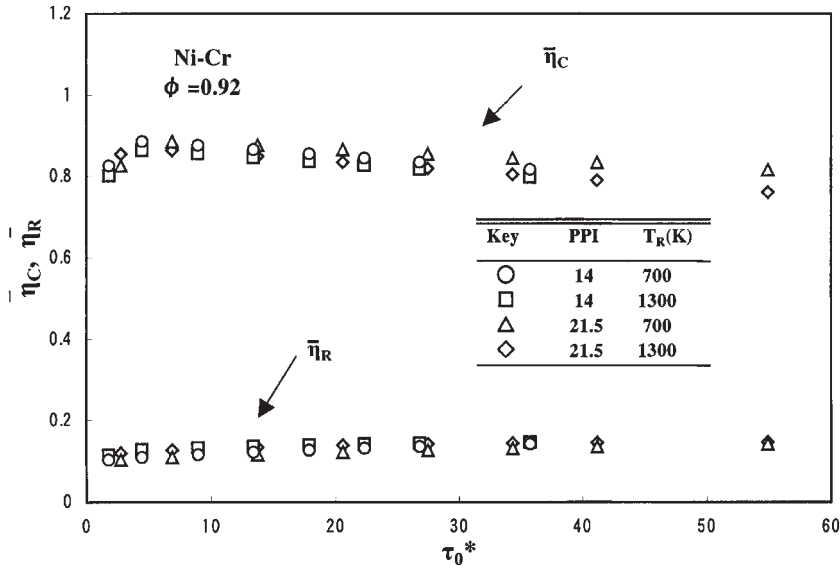


Figure 6.22 Variations in the mean conversion efficiency and the mean slab reflectance of a Ni-Cr open-cellular porous heat shield against the optical thickness.

examine the effect of several parameters including kinds of porous material, PPI and equivalent blackbody temperature characterizing incoming radiation on the mean conversion efficiency $\bar{\eta}_C$ and the mean slab reflectance $\bar{\eta}_R$, numerical simulations are performed for two kinds of Ni-Cr foam, i.e. NC#02 ($\phi = 0.92$ and PPI = 14), and NC#03 ($\phi = 0.92$ and PPI = 21.5), and two kinds of cordierite-alumina foam, i.e. CA#06 ($\phi = 0.89$ and PPI = 6) and CA#20 ($\phi = 0.89$ and PPI = 20). Since air velocity is varied from 0.25 and 5 m s⁻¹, the mean conversion efficiency $\bar{\eta}_C$ is defined by an arithmetic mean of $\bar{\eta}_C$ at $u = 0.25$ and 5 m s⁻¹ and the mean slab reflectance $\bar{\eta}_R$ is defined by an arithmetic mean of $\bar{\eta}_R$ at $u = 0.25$ and 5 m s⁻¹. Results for $\bar{\eta}_C$ and $\bar{\eta}_R$ are shown in Figures 6.22 and 6.23. The horizontal axis denotes the optical thickness defined as $\beta^* x_0$. As seen from these figures, $\bar{\eta}_C$ and $\bar{\eta}_R$ are slightly influenced by an equivalent blackbody temperature of incoming radiation T_R (K), but the observed relative difference between the results for different T_R is less than $\pm 15\%$ at the worst and thus can be disregarded. $\bar{\eta}_R$ increases with τ_0^* and almost levels off at $\tau_0^* \approx 5$, while $\bar{\eta}_C$ increases with τ_0^* and takes a maximum at $\tau_0^* \approx 5$. It is also found from relations between η_T and τ_0^* , which are not presented here, that η_T increases rapidly with τ_0^* and is saturated at a constant value in the region of τ_0^* less than 5. Comparison between Figures 6.22 and 6.23 reveals that $\bar{\eta}_C$ of the cordierite-alumina porous plate is less than that of the Ni-Cr porous plate, while the reverse is the case for $\bar{\eta}_R$. This is clear from the fact that the hemispherical reflectivity of cordierite-alumina is greater than that of Ni-Cr: the Ni-Cr porous plate with $\tau_0^* \approx 5$ absorbs about 90% of the incoming radiation, while the cordierite-alumina porous plate

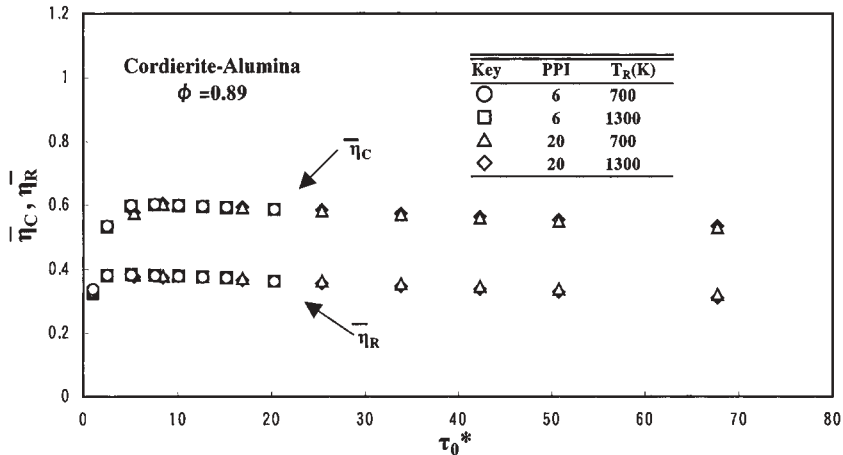


Figure 6.23 Variations in the mean conversion efficiency and the mean slab reflectance of a cordierite-alumina open-cellular porous heat shield against the optical thickness.

with the same optical thickness absorbs about 60% of the incoming radiation. Moreover, it may be concluded that the transpiration cooling system using an open-cellular porous plate should be designed so as to realize $\tau_0^* \approx 5$.

6.7

Conclusions and Recommendations

The major conclusions and recommendations of the present chapter are summarized as follows:

1. The Schuetz–Glicksman formula in predicting the effective thermal conductivity of an open-cellular porous medium by conduction alone is the most accurate among the formula examined here.
2. Use of analytical formulas for the radiative properties derived by Kamiuto are recommended.
3. A correlation for the volumetric heat transfer coefficients obtained by Kamiuto and Yee is useful, but it should be noted that this correlation includes the effects of axial thermal dispersion and/or fluid conduction.
4. The proposed empirical formulas for the permeability and inertial coefficient are useful.
5. Radiative transfer through an open-cellular porous material can be treated accurately utilizing transfer-theoretical approach based on Kamiuto's radiative property model.

6. Recommended analytical formulas for the thermal, radiative and fluid mechanical properties can be used accurately in theoretically analyzing composite heat transfer in open-cellular porous media at high temperatures.
7. The P_1 approximation is quite accurate in predicting composite heat transfer in open-cellular porous media.

Nomenclature

A	parameter
A', B'	Eqs. (6.36)
c_{ps}	specific heat of solid
c_{pf}	specific heat of fluid at constant pressure
D_c	mean diameter of Dul'nev's unit cells
D_m	actual mean pore diameter
D_n	nominal cell diameter
D_p	equivalent strut diameter
d_p	mean sphere diameter
$E(k^2)$	complete elliptic integral of the second kind
F	inertial coefficient
f	numerical factor ($=1/3$)
G	incident radiation
$\tilde{g}$	asymmetry factor
$\tilde{g}_d$	asymmetry factor of the surface scattering phase function of a diffuse sphere ($= -4/9$)
h_v	volumetric heat transfer coefficient between the fluid and solid phases
I	intensity of radiation
I_b	blackbody intensity
K	permeability
$\underline{\underline{K}}_d$	thermal dispersion tensor
$\underline{\underline{K}}_{cf}$	effective thermal conductivity tensor of the fluid phase
$\underline{\underline{K}}_{cs}$	effective thermal conductivity tensor of the solid phase
$\underline{\underline{K}}_{eff}$	effective thermal conductivity tensor of a porous medium
k_{da}	axial thermal dispersion conductivity
k_{dl}	lateral thermal dispersion conductivity
$k_{eff,c}$	stagnant effective thermal conductivity of a porous medium by conduction alone
$\bar{k}_{eff,c}$	mean effective thermal conductivity by conduction alone
$\bar{k}_{eff,t}$	mean total effective thermal conductivity
k_f	thermal conductivity of fluid
k_s	thermal conductivity of solid
l_i	characteristic length of a porous medium
Nu_i	Nusselt number defined by $h_v l_i^2 / k_f$

P	pressure
$P(\mu, \mu')$	azimuthally averaged scattering phase function
$P_n(\mu)$	Legendre function
PPI	pores per inch
q_c	conductive heat flux
$q_{R\gamma}$	component of the radiative heat flux vector
$q_{R,f}$	radiative heat flux from an environment
$\mathbf{q}_R$	radiative heat flux vector
q_t	total heat flux
$\mathbf{v}$	position vector
Re_p	Reynolds number ($=u_m D_p / \nu_f$)
T	temperature
T_b	blackbody temperature
T_R	equivalent radiation source temperature
T_∞	ambient temperature
t	time
u	axial velocity
u_m	mean velocity
$\mathbf{V}$	Darcian velocity vector
w	dimensionless width of a strut with a square cross section
x	axial coordinate
x_0	(or γ_0) thickness of a porous plate
y	depth coordinate
β	extinction coefficient
γ_{da}	axial dispersion coefficient
γ_{dl}	lateral dispersion coefficient
δ	quantity defined by $T/1000$ (K)
ε	emissivity
η_C	conversion efficiency
η_T	temperature efficiency
η_R	slab reflectance
θ	dimensionless temperature
μ	direction cosine
μ_f	viscosity
ν_f	kinematic viscosity
π	ratio of the circumference of a circle to its diameter
ρ	reflectivity
ρ_f	density of fluid
σ	Stefan–Boltzmann constant
σ_a	absorption coefficient
σ_s	scattering coefficient
ϕ	porosity
ω	albedo
Ω	direction vector

Subscripts

d	downstream
f	fluid
H	hot boundary or hemispherical
L	cold boundary
m	mixture
N	normal
s	solid
T	(or t) total
u	upstream
w	wall
v	frequency
∞	ambient

Superscript

*	scaled quantity
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Miscellaneous

∇	gradient
∇^2	Laplacian
$\mathbf{V} \cdot$	divergence
$\bar{z}$	mean value of z

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7

Thermal Conduction Through Porous Systems*Ramvir Singh*

7.1

Introduction

Heat transfer through porous materials continues to be a major field of interest to engineers and scientific researchers, as well as developers and manufacturers, due to the numerous applications of these materials in different branches of science and engineering. Study of heat conduction to design high-tech thermal devices to accomplish certain engineering objectives is of extreme importance. It is also important to consider economic factors while designing any such equipment. Insulation is commonly used to reduce thermal loss or gain from a device. Therefore, proper heat conduction analysis will be the first step in designing heating or air conditioning equipment for a building, energy saving devices, lightweight constructions and high-temperature furnaces. Detailed study of thermal conductivity of metal foams is needed to design aircraft wings. In semiarid zones, thermal study of walls and roofs will be useful as they contain air pockets in their structure [1].

Other areas and applications where the study of heat conduction becomes mandatory are extraction of geothermal energy, solar ponds, food preservation, building environment and architecture, heat pumps, microstructure electronics, global warming, power plants, energy consumption in buildings, etc. In order to calculate heat dissipation in activities like underground nuclear explosions and heating losses from earth due to geothermal gradient, values of the thermal parameters for the materials used are required. For instance, values of thermal parameters of soil need to be calculated for laying buried cables and hot water pipes.

Thermophysical parameters such as the thermal conductivity (λ), thermal diffusivity (κ), heat storage coefficient (β) and heat capacity (C) are the main parameters which govern the heat transport in multiphase systems. By analyzing any two of these parameters, one can do a thermophysical study of the system. The thermal conductivity of a material is represented by Fourier's [2] equation as

$$q = -\lambda_e \frac{dT}{dz}$$

where λ_e = effective thermal conductivity of the system, dT/dz = temperature gradient and q = amount of heat passing through unit area.

The thermal diffusivity κ represents the speed of propagation of heat in a medium during change of temperature with time. If thermal diffusivity of a system is high, then the propagation of the heat in medium will be fast. The effective value of the thermophysical parameter will lie in between the same parameters of the constituent phases.

The thermal conductivity of a heterogeneous material is normally defined as the heat flux divided by the temperature drop per unit length. Foams are quite heterogeneous structures with pores and membranes of different shapes and cross-sections. Metal foams are a relatively new class of structural materials and offer a variety of applications in lightweight construction and crash energy management. These days, aluminum alloy foams are on the verge of being used in industrial applications. Evaluation of the effective thermal conductivity (λ_e) of porous materials is also important for a wide range of engineering problems. Heat conduction in porous materials is usually described macroscopically by averaging the microscopic heat transfer process over a representative elementary volume [3]. Heat conduction in porous materials is based largely on mixture theory, assuming local thermal equilibrium within solid and fluid phases, so that the heat transfer process in the two phases can be lumped into a process described by a single heat conduction equation.

The thermal conductivity of a porous material depends on various parameters such as the thermal properties of constituent phases and the microstructural parameters which include the volume fractions of constituent phases, the geometrical distribution of the phases, the size and distribution of particles and the geometry of pore structure [4]. These parameters become more important where the variations of pressure, moisture content and temperature occur.

Porous materials are generally of two types: cellular and granular. A granular material is a two-phase system in which the fluid phase is continuous and solid phase is dispersed; in cellular materials, the solid phase is continuous and the fluid phase is dispersed. Sands, powders, porous rocks and wool fall into the category of granular materials. A granular material has a lower thermal conductivity than a cellular one of the same material, which makes it a better insulator. In granular materials, pores are usually very small and the drop in temperature will not reach 100°C; then thermal convection and thermal radiation can be neglected. Moisture migration is also very much less in these materials, which reduces the possibility of mass transfer.

In Section 7.2 we discuss theoretical models for calculation of the thermal conductivity while in Section 7.3 experimental techniques for the measurement of the same are discussed.

7.2

Theoretical Models

7.2.1

Models for Thermal Conductivity

Heat conduction through porous media depends on the structure of the material and the thermal conductivity of each phase. A variety of methods, exact, approximate and purely numerical, to evaluate the effective thermal conductivity have been derived by different researchers for different systems. New theoretical models are still needed to support the new kinds of systems which are coming up due to present day requirements and new technological developments. Theoretical models developed can mainly be classified on the basis of following approaches:

- **Field approach.** It is worth noting that magnetic permeability, dielectric constant, electrical conductivity and thermal conductivity are described by the Laplace equation. The solutions of the Laplace equation for these properties are mathematically identical. Therefore a configuration that bears some relationship with the microstructure of the system is assumed and the disturbance due to structural elements to the linear flow of heat is determined. In the derivation of resistor approach models, it was assumed that the lines of flux are straight. Actually, the flux lines form concentrated or rarefied field regions in the vicinity of the dispersed grains. The degree of concentration or rarefaction depends upon the ratio of thermal conductivity of constituent phases. Knowing the conductivity of the phases, it is possible to derive the relative flux density inside or outside the particle. With this knowledge, the effective thermal conductivity of the mixture can then be calculated [5–10].
- **Resistor approach.** In this approach [11–19] the continuous and dispersed phases are treated like parallel slabs which behave as thermal resistors to the heat flux (as resistors obey Ohm's law) and flux lines follow a straight-line path. In different models different configurations of slabs have been considered.
- **Phase averaging approach.** In this approach [20–23], the effective thermal conductivity is obtained as an average property of the mixture of constituent phases. In each phase the volume average of the temperature gradient is taken and this is further related to the average temperature of the medium.

In the following discussion, a comprehensive and systematic effort is made to incorporate most of the popular models developed for calculation of the effective thermal conductivity of porous materials and discuss their limitations.

Maxwell [5] gave a model for the prediction of the effective thermal conductivity by assuming random size spheres dispersed into a continuous medium. The value of effective thermal conductivity for such a system can be represented as

$$\lambda_e = \lambda_c \frac{[2\lambda_c + \lambda_d - 2\phi_d(\lambda_c - \lambda_d)]}{[2\lambda_c + \lambda_d + \phi_d(\lambda_c - \lambda_d)]} \quad (7.1)$$

where λ_c is the thermal conductivity of the continuous phase, λ_d is the thermal conductivity of dispersed phase and ϕ_d is the volume fraction of dispersed phase, respectively.

Fricke [6] and Burgers [7] modified the Maxwell model for particles having ellipsoidal shape. The expression obtained by Fricke and Burgers is

$$\lambda_e = \frac{\lambda_c \phi_c + \lambda_d (1 - \phi_c) F}{\phi_c + (1 - \phi_c) F} \quad (7.2)$$

where

$$F = \frac{1}{3} \sum_{i=1}^3 \left[1 + \left\{ \left(\frac{\lambda_d}{\lambda_c} \right) - 1 \right\} g_i \right]^{-1}$$

and $\sum_{i=1}^3 g_i = 1$. They assumed that particles were noninteracting. F is the ratio of the average temperature gradients in the two phases and g_i are the semi-principal axes of the ellipsoid.

De Vries [8] in his derivation of the effective thermal conductivity used $g_1 = g_2 = 1/8$ and $g_3 = 3/4$. This implies that the two minor axes of the ellipsoid are the same and the major axis is three times that of the minor axis.

Bruggeman [9] used Maxwell's model for cylindrical particles. He obtained an expression for the effective thermal conductivity in the following form:

$$\lambda_e = \frac{\lambda_c \left[1 - \left(1 - \frac{\lambda_d}{\lambda_c} \right) \frac{2}{3} \phi_d \delta \right]}{[1 + (\delta - 1) \phi_d]} \quad (7.3)$$

Here ϕ_d is the fractional volume of inclusions and δ is determined from λ_c and λ_d . The value of δ is

$$\frac{3\lambda_c}{2\lambda_c + \lambda_d} \quad \text{for spherical particles}$$

$$\frac{5\lambda_c + \lambda_d}{3(\lambda_c + \lambda_d)} \quad \text{for cylindrical particles}$$

and

$$\frac{\lambda_c + 2\lambda_d}{3(\lambda_d)} \quad \text{for plates and scales}$$

Rayleigh [10] assumed that particles are spherical in shape and they are arranged in a cubical array. The expression for the effective thermal conductivity given by Rayleigh is

$$\lambda_e = \frac{\lambda_c [1 - 2\phi.k - 1.65(\phi)^{10/3} Ak]}{[1 + \phi.k - 1.65(\phi)^{10/3} Ak]} \quad (7.4)$$

where

$$k = \frac{(\lambda_c - \lambda_d)}{(2\lambda_c + \lambda_d)} \quad \text{and} \quad A = \frac{(3\lambda_c - 3\lambda_d)}{(4\lambda_c + 3\lambda_d)}$$

Rayleigh's model is so rigid and artificial that it does not predict λ_e of mixtures in practical cases.

Wiener [11] developed a model based on the resistors concept. This concept was a turning point in theoretical models for the effective thermal conductivity. Wiener considered the system to be made of alternate layers of solid and fluid in the form of slabs. These slabs can be arranged in different configurations with respect to the direction of heat flux.

- **Parallel configuration.** In this configuration the plane of equivalent slabs is parallel to the direction of heat flow i.e. the two phases are thermally parallel to the heat flux. The effective thermal conductivity for parallel configuration $\lambda_{\parallel}$ can be expressed as the weighted arithmetic mean of the conductivities of the solid and fluid phases and is written as

$$\lambda_{\parallel} = [\phi\lambda_f + (1-\phi)\lambda_s] \quad (7.5)$$

The parallel configuration offers minimum insulation resulting into maximum value of effective thermal conductivity.

- **Perpendicular configuration.** When the direction of heat flow is perpendicular to the plane of slabs, then it offers maximum insulation and the value of the effective thermal conductivity is a minimum. In this configuration, the constituent phases are thermally in series with the direction of heat flow. Effective thermal conductivity in this case is represented as $\lambda_{\perp}$ and is given by the weighted harmonic mean of the conductivities of the constituent phases:

$$\lambda_{\perp} = \left[\frac{\phi}{\lambda_f} + \frac{(1-\phi)}{\lambda_s} \right]^{-1} \quad (7.6)$$

The above equations for the effective thermal conductivity are the limiting formulas for all possible conductivities of phases for a given value of the porosity ϕ .

Later, Woodside and Messmer [12] analyzed these relations more critically and concluded that for both the distributions (parallel and perpendicular configurations), one should have

$$\left[\frac{d\lambda_e}{d\lambda_s} \right]_{\lambda_s=\lambda_f} = (1-\phi) \quad (7.7)$$

Hence Eq. (7.7) should be satisfied by different relations for the effective thermal conductivity applicable to different kinds of distributions.

In a dispersed system, the conductivity of the aggregate depends on the relative magnitude of the conductivity of the continuous and dispersed phases. This

information is important, particularly when there is a substantial difference between the conductivities of the two phases. Both the schemes [11] of phase distribution assume either ideal contact (in the case of $\lambda_{||}$) or no contact of phases at all (as in the case of $\lambda_{\perp}$) and as such these schemes do not reflect the true state of the phase distribution in a natural system.

In this series, Bernshtein [13] gave the following relation assuming the material is in the form of plates placed in a chessboard-like order:

$$\lambda = \lambda_f \left[\frac{4(1-\phi)}{1 + \frac{\lambda_f}{\lambda_s}} + 2(\phi-1) \right] \quad \phi \geq 0.5$$

and

$$\lambda = \lambda_f \left[\frac{4(1-\phi)}{1 + \frac{\lambda_f}{\lambda_s}} + \frac{\lambda_s}{\lambda_f} (1-2\phi) \right] \quad \phi \leq 0.5 \quad (7.8)$$

These schemes gave a considerable improvement over Wiener's model, yet are quite far from the realistic structure of granular materials.

Lichtenecker [14] has given an empirical relation to express the behavior of a two-phase system that has been named the "logarithmic law of mixing". The expression for the effective thermal conductivity as per this law can be written as

$$\log(\lambda_e) = \phi_f \log(\lambda_f) + \phi_s \log(\lambda_s) \quad (7.9)$$

where the respective conductivities and corresponding volume fractions are represented by subscripts s and f. The value of λ_e of a mixture should be found between upper and lower limiting values for distinctly dispersion-type of systems. This equation can also be written in a different form as

$$\lambda_e = (\lambda_f)^{\phi_f} \cdot (\lambda_s)^{\phi_s} \quad (7.10)$$

Equation (7.10) is intended only for particles having two-directional randomization and oriented in the third direction. For particles having three-directional randomization, Bruggeman [9] has extended Lichtenecker's relation as

$$\lambda_e = \lambda_f^{\phi_f (1+k\phi_s)} \lambda_s^{\phi_s (1+k\phi_f)} \quad (7.11)$$

where

$$k = \frac{3}{2} \left(\frac{\lambda_s - \lambda_f}{(2\lambda_s + \lambda_f)(\lambda_s + \lambda_f)} \right)$$

Expression (7.10) can be extended to number n of phases and is written as

$$\log \lambda_e = \sum_{i=1}^n \phi_i \log(\lambda_i) \quad (7.12)$$

Russel [15] developed a model for predicting the effective thermal conductivity by assuming that the cubes of one phase are arranged in a cubic array into other phase (Figure 7.1). If the dispersed cubes are solid and the continuous phase is fluid, then

$$\lambda_e = \frac{\lambda_f \left[(\phi_s)^{\frac{2}{3}} + \left(\frac{\lambda_f}{\lambda_s} \right) \left(1 - \phi_s^{\frac{2}{3}} \right) \right]}{\left[(\phi_s)^{\frac{2}{3}} - \phi_s + \left(\frac{\lambda_f}{\lambda_s} \right) \left(1 + \phi_s - \phi_s^{\frac{2}{3}} \right) \right]} \quad (7.13)$$

In the opposite case, when the dispersed phase is fluid and the solid phase is continuous one, then Eq. (7.13) will be modified as

$$\lambda_e = \frac{\lambda_s \left[(\phi_f)^{\frac{2}{3}} + \left(\frac{\lambda_s}{\lambda_f} \right) \left(1 - \phi_f^{\frac{2}{3}} \right) \right]}{\left[\phi_f^{\frac{2}{3}} - \phi_f + \left(\frac{\lambda_s}{\lambda_f} \right) \left(1 - \phi_f - \phi_f^{\frac{2}{3}} \right) \right]} \quad (7.14)$$

For porous materials, Ribaud [16] later proposed an equation by assuming that the pores are joined in a cubical manner resulting into an expression for λ_e as

$$\lambda_e = \lambda_s (\phi_s)^{\frac{2}{3}} + \lambda_f (\phi_f)^{\frac{1}{3}} \quad (7.15)$$

A natural system, however, is not as simple as predicted by these formulas, for there are always contacts among the particles. Ignoring this important fact restricts the applicability of these relations to natural systems.

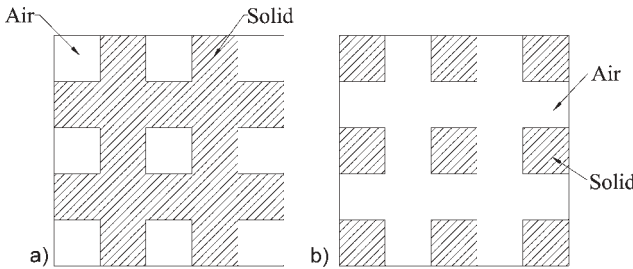


Figure 7.1 Russel's model for the effective thermal conductivity of porous media: (a) cubes of air with solid substance in between; (b) cubes of solid separated by air spaces.

Powers [24] has made a survey of methods for calculating the thermal conductivity of aggregates of almost any type. He has shown that when there is an increase in porosity of the dispersed phase to nearly 50%, the dispersed phase can no longer be regarded as discontinuous phase but it behaves as a continuous phase. In several cases having concentrations between 25 and 75%, both phases can be a dispersed phase. Such systems are termed as mixtures. Powers concluded (for mixtures) that the particles are no longer distributed systematically, but may be elongated in one or more directions and oriented randomly.

Bogomolov [25] developed a similar kind of expression by taking into account that solid spheres are packed into a tetrahedral packing. The resultant expression so obtained has been extensively used for determination of the effective thermal conductivity:

$$\lambda_e = 3\pi\lambda_f \ln \left[\frac{0.43 + 0.31\phi}{\phi - 0.26} \right] \quad (7.16)$$

Assad [26] gave an expression for effective thermal conductivity of sandstone rocks. His relation was an empirical one:

$$\lambda_e = \lambda_s \left[\frac{\lambda_f}{\lambda_s} \right]^{B\phi} \quad (7.17)$$

where B is a constant and is related to the characteristics of sandstone.

More developments in the expressions of heat conduction took place with the new models and formulations resulting in new kinds of applications.

Kunni and Smith [27] took a practical approach and proposed a relation for effective thermal conductivity of loose granular materials as

$$\lambda_e = \lambda_f \left[\frac{\phi + \beta(1-\phi)}{e + (2\lambda_f/3\lambda_s)} \right] \quad (7.18)$$

where β is an adjustable parameter ranging between 0.9 and 1, and

$$e = e_2 + \left[\frac{\phi - 0.259}{0.217} \right] (e_1 - e_2) \quad (7.19)$$

Here e_1 and e_2 are dependent on values of ϕ for loose and compact packing. When $\phi < 0.259$ then $e = e_2$ and when $\phi > 0.476$ then $e = e_1$.

Woodside and Messmer [12] proposed three modes of heat conduction using the resistor approach. They assumed that there is solid to solid conduction, fluid to fluid conduction and solid to fluid conduction and vice versa. Their expression for the effective thermal conductivity is

$$\lambda_e = \alpha \left[\frac{\lambda_s \lambda_f}{\lambda_s(1-\gamma) + \lambda_f \gamma} \right] + \beta \lambda_s + \delta \lambda_f \quad (7.20)$$

where $\alpha + \beta + \gamma = 1$ and $\alpha\gamma + \beta = (1 - \phi)$. Here α , β and γ are parameters for cube formation and δ is the reciprocal of formation factor F . Thus

$$\delta = \frac{1}{F} = \phi - 0.03$$

The estimation of the effective thermal conductivity using a curve-fitting technique has been presented by Sugawara and co-workers [28,29]. The expression given by them for the measurement of λ_e of soil, rocks and other granular materials is

$$\lambda_e = [(1-A)\lambda_s + A\lambda_f] \quad (7.21)$$

where

$$A = \frac{2^n}{(2^n - 1)} [1 - (1 + \phi)^{-n}]$$

and n represents an empirical number.

Maxwell's model has been extended by Brailsford and Major [30] for a wide range of dispersions. In this model, the constituent phases are mixed in a definite proportion for a two-phase system. This mixture is then embedded in a random mixture of the same two phases having conductivity equal to the average value of the conductivity of the two-phase system. Thus the thermal conductivity of such a three-phase system can be determined as

$$\lambda_e = \frac{\left[\lambda_c \phi_c + \lambda_{d1} \phi_{d1} \left(\frac{3\lambda_c}{2\lambda_c + \lambda_{d1}} \right) + \lambda_{d2} \phi_{d2} \left(\frac{3\lambda_c}{2\lambda_c + \lambda_{d1}} \right) \right]}{\left[\phi_c + \phi_{d1} \left(\frac{3\lambda_c}{2\lambda_c + \lambda_{d1}} \right) + \phi_{d2} \left(\frac{3\lambda_c}{2\lambda_c + \lambda_{d1}} \right) \right]} \quad (7.22)$$

where subscripts c and d represent continuous and dispersed phases, respectively.

Chaudhary and Bhandari [17] extended the Lichtnecker model by considering the series and parallel resistors concept for a two-phase system. The random distribution of series and parallel resistors is represented by an empirical factor n , which denotes the probability of orientation of parallel resistors in the direction of heat flow. The resultant expression for the effective thermal conductivity is given by

$$\lambda_e = (\lambda_{||})^n (\lambda_{\perp})^{1-n} \quad (7.23)$$

where

$$\lambda_{||} = [\phi\lambda_f + (1-\phi)\lambda_s], \quad \lambda_{\perp} = \left[\frac{\phi}{\lambda_f} + \frac{(1-\phi)}{\lambda_s} \right]^{-1} \quad \text{and} \quad n = \frac{k(1-\log \phi)}{\log \left[\phi(1-\phi) \left(\frac{\lambda_s}{\lambda_f} \right) \right]}$$

where k is an empirical constant.

In this vein Cheng and Vachon [31] proposed a model for randomly distributed particles in a continuous phase. Their model is represented by the equation for the effective thermal conductivity as

$$\frac{1}{\lambda_e} = 2 \int_0^{\frac{B}{2}} \left[\frac{dx}{\lambda_c + B(\lambda_d - \lambda_c) - Cx^2(\lambda_d - \lambda_c)} \right] + \frac{1-B}{\lambda_c} \quad (7.24)$$

where

$$B = \left[\frac{3\phi}{2} \right]^{\frac{1}{2}}, \quad C = 4 \left[\frac{2\phi}{3} \right]^{\frac{1}{2}} \quad \text{and} \quad \phi = \phi_d$$

Here x is the dimension of dispersed phase along the x -axis. This expression was found to be suitable for values of $\phi \leq 0.667$.

Later on, a bound technique for determination of λ_e with lower and upper bounds came into the picture due to the lack of a general expression. The technique estimates the closest optimum value of λ_e . A general set of bounds has been presented by Hashin and Strikman [32] incorporating a variational principle for physically realizable particles or particles having cylindrical geometry as

$$\lambda_f + \frac{\phi_s}{\left[\frac{1}{(\lambda_s - \lambda_f)} + \frac{\phi_f}{3\lambda_f} \right]} < \lambda_e < \lambda_s + \frac{\phi_f}{\left[\frac{1}{(\lambda_f - \lambda_s)} + \frac{\phi_s}{3\lambda_s} \right]} \quad (7.25)$$

Prager [33] presented a solution for the bounds for particles having cylindrical geometry using λ_e values of some other materials whose conductivity ratios are the same but the constituent phases may be different. A set of bounds have been derived by Schulgasser [34] for fibrous reinforced materials applying symmetry considerations. His bounds are expressed as

$$\lambda_s \lambda_f \left[\lambda_{||} - \frac{\phi \left\{ \frac{(1-\phi)}{2} (\lambda_f - \lambda_s)^2 \right\}}{\phi \frac{(1-\phi)}{2} \lambda_{||} + (\lambda_s - \lambda_f) I_1} \right]^{-1} < \lambda_e < \lambda_s \lambda_f \left[\lambda_{||} - \frac{\phi \left\{ \frac{(1-\phi)}{2} (\lambda_s - \lambda_f)^2 \right\}}{\phi \frac{(1-\phi)}{2} \lambda_{||} + (\lambda_f - \lambda_s) I_2} \right] \quad (7.26)$$

where I_1 and I_2 are geometry-dependent factors. These can be evaluated considering a statistically three-dimensional isotropic medium.

Using statistical properties of materials and generalized functions, Hori [35] developed a model for effective constants of a heterogeneous medium. Under specific conditions his theory yields Weiner [11] and Hashin and Strikman [32] bounds.

Kumar and Chaudhary [18] developed a model by presenting an empirical bound for effective thermal conductivity based on random distribution of series

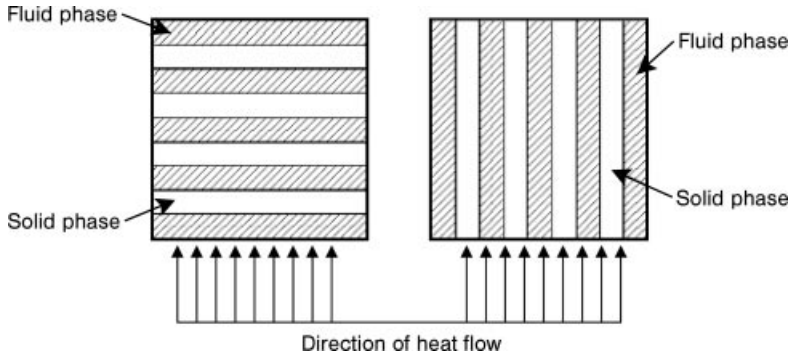


Figure 7.2 Model of dispersed resistors giving extreme conductivity values ($\lambda_{\parallel}$ and $\lambda_{\perp}$).

and parallel resistors (Figure 7.2). Their expression for λ_e with lower and upper bound is written as

$$\left[\lambda + \phi_f(1-\phi_f) \{ \lambda_f \lambda_s e^{\omega(2\phi_f-1)} \}^{\frac{1}{2}} \right] < \lambda_e < \left[\lambda - \phi_f(1-\phi_f) \{ \lambda_f \lambda_s e^{\omega(2\phi_f-1)} \}^{\frac{1}{2}} \right] \quad (7.27)$$

where

$$\lambda = \lambda_s(1-\phi_f)e^{\omega\phi_f} + \lambda_f\phi_f e^{-\omega(1-\phi_f)}$$

and

$$\omega = \left[\frac{\lambda_f}{\lambda_s} - 1 \right] \quad \text{for } \lambda_f < \lambda_s; \quad \omega = \left[1 - \frac{\lambda_s}{\lambda_f} \right] \quad \text{for } \lambda_f > \lambda_s$$

This model was further modified by Pande et al. [36]. Their proposed model is written mathematically in terms of bounds as

$$\frac{1}{(e^b-1)} [(\lambda_f-\lambda_s)e^{b\phi} + \lambda_s e^b - \lambda_f] > \lambda_e > \frac{1}{(e^a-1)} [(\lambda_f-\lambda_s)e^{a\phi} + \lambda_s e^a - \lambda_f] \quad (7.28)$$

where

$$a = \left[\frac{\lambda_f - \lambda_s}{(\lambda_s \lambda_f)^{1/2}} \right] \quad \text{and} \quad b = \left[\frac{\lambda_f^2 - \lambda_s^2}{\lambda_f^2 + \lambda_s^2} \right]$$

Zimmerman [37] modified the Fricke relation for fluid-saturated rocks having different types of pores. For very small porosity, Fricke [6] showed that the effective thermal conductivity is given as

$$\frac{\lambda_e}{\lambda_s} = (1-\beta\phi) \quad (7.29)$$

where

$$\beta = \frac{1-r}{3} \left[\frac{4}{2 + (r-1)M} + \frac{1}{1 + (r-1)(1-M)} \right]$$

Here $r = \lambda_f/\lambda_s$ and M is a factor that depends on aspect ratio of the pore. Zimmerman [37] gave more interesting and useful analytical expressions for β for three limiting cases:

$$\text{For thin cracks} \quad \beta \rightarrow \frac{(1-r)(1+2r)}{3r}$$

$$\text{For spherical pores} \quad \beta \rightarrow \frac{3(1-r)}{2+r}$$

$$\text{For needle-like pores} \quad \beta \rightarrow \frac{(1-r)(5+r)}{3(1+r)}$$

Recently, Torquato and Rintoul [38] developed rigorous bounds on the effective thermal conductivity of dispersions that are given in terms of the phase contrast between the inclusion and matrix, the interface strength, volume fraction and higher order morphological information, including morphological information. His bounds give very accurate predictions of λ_e for dispersions of metallic particles in epoxy matrices. The upper and lower bounds are

$$\frac{\lambda_e}{\lambda_f} \leq D_U(C) = 1 + (\alpha + 3C - 1)\phi_s - \frac{E_U}{F_U} \quad (7.30)$$

where

$$E(U) = \phi_s \left\{ \phi_f \left[C(5 - 5\alpha - 6C) - (\alpha - 1)^2 \right] - 3C \right\}^2$$

and

$$\begin{aligned} F(U) = & 6C + (\alpha - 1 + 2C)^2 + [3\phi_f + (\alpha - 1)(2\xi_s\phi_f + \phi_f^2)] \\ & + C\phi_s(\alpha - 1 + 2C)^2 \left[\frac{16}{9} + 3\phi_s(1 + \phi_2) \right] \\ & + 3C[\phi_f(\alpha - 1 + 2C) + 1]^2 \end{aligned}$$

$$\frac{\lambda_e}{\lambda_f} \geq D_L(C) = \left\{ 1 + \left(\frac{1}{\alpha} - 1 \right) \phi_s - \frac{E_L}{F_L} \right\}^{-1} \quad (7.31)$$

where

$$E_L = \phi_s [2\phi_f(\alpha - 1 + 2C)(\alpha - 1) + 6C]^2$$

and

$$F_L = 6\alpha^2 \left\{ 3C + 6C^2 + \phi_s [(\alpha-1)^2 - 4C^2] \right\} + (\alpha-\alpha^2) \left\{ 4 \left[\phi_f (\alpha-C-1) - 3C\phi_s \right]^2 + 2\xi_s \phi_f (\alpha-1+2C)^2 \right\}$$

The parameters C , α and ξ are defined in Torquato and Rintoul [38].

Pande et al. [20] also gave an expression for the prediction of λ_e of a granular system by considering regular geometry of the dispersed phase:

$$\lambda_e = \lambda_f \left[1 + 3.7396 \left(\frac{\lambda_s - \lambda_f}{\lambda_s + 2\lambda_f} \right) \phi^{2/3} \right] \quad (7.32)$$

This represents the interaction between gas and solid particles up to sixth order for two-phase systems. The higher orders are negligible due to their very small contribution. According to the ratios of thermal conductivities of the constituents, the above relation is represented as

$$\lambda_e = \lambda_f \left[1 + 3.844(\phi)^{\frac{2}{3}} \right] \quad \text{for } \lambda_s \gg \lambda_f$$

$$\lambda_e = \lambda_f \left[1 - 1.154(\phi)^{\frac{2}{3}} \right] \quad \text{for } \lambda_s \ll \lambda_f$$

$$\lambda_e = \lambda_f \left[1 + 2.307 \left(\frac{\lambda_s - \lambda_f}{\lambda_s + 2\lambda_f} \right) (\phi)^{\frac{2}{3}} \right] \quad \text{for } \lambda_s = \lambda_f$$

Pande et al. [21] further modified these equations for an effective continuous medium as

$$\lambda_e = 0.6132(\lambda_f \lambda_s)^{\frac{1}{2}} \left\{ 1 - 1.154(\psi_f)^{\frac{2}{3}} \right\} \quad \text{for } \psi_f = |\phi_f - 0.5|$$

and

$$\lambda_e = 0.6132(\lambda_f \lambda_s)^{\frac{1}{2}} \left\{ 1 + 3.844(\psi_s)^{\frac{2}{3}} \right\} \quad \text{for } \psi_s = |\phi_s - 0.5| \quad (7.33)$$

Here ϕ_s and ϕ_f are the volume fractions of solid and fluid phases.

Beniwal et al. (36) extended the work of Pande et al. for statistically homogeneous and regular multiphase systems. The solution of Poisson's equation was used for effective neighboring interactions and modified field which thereafter yields the effective thermal conductivity of multiphase systems as

$$\lambda_e = \lambda_c \left[1 + 3.844\phi_c^{-\frac{1}{3}} \left\{ \left(\frac{\lambda_{d_1} - \lambda_c}{\lambda_{d_1} + 2\lambda_c} \right) \phi_{d_1} + \left(\frac{\lambda_{d_2} - \lambda_c}{\lambda_{d_2} + 2\lambda_c} \right) \phi_{d_2} \right\} \right] \quad (7.34)$$

When there is a very dilute dispersion of both the phases, the interactions may not spread over a large distance. Therefore, Eq. (7.34) has the form

$$\lambda_e = \lambda_c \left[1 + 3.489\phi_c^{-1/3} \left\{ \left(\frac{\lambda_{d1} - \lambda_c}{\lambda_{d1} + 2\lambda_c} \right) \phi_{d1} + \left(\frac{\lambda_{d2} - \lambda_c}{\lambda_{d2} + 2\lambda_c} \right) \phi_{d2} \right\} \right] \quad (7.35)$$

Hadley [23] in his contribution for the determination of λ_e gave a model by taking into account the average of temperature field over different phases. The expression so obtained for λ_e is written as

$$\lambda_e = \frac{\lambda_f \left[(1-\phi)F + \frac{\lambda_s}{\lambda_f} \{1-(1-\phi)F\} \right]}{\left[1 - \{(1-\phi)(1-F)\} + \frac{\lambda_s}{\lambda_f} (1-\phi)(1-F) \right]} \quad (7.36)$$

The value of F lies between 0 and 1.

Equation (7.36) for λ_e is modified for packed metal powders as

$$\frac{\lambda_e}{\lambda_f} = (1-\beta) \frac{\left[(1-\phi)F_0 + \frac{\lambda_s}{\lambda_f} \{1-(1-\phi)F_0\} \right]}{\left[1 - \{(1-\phi)(1-F_0)\} + \frac{\lambda_s}{\lambda_f} (1-\phi)(1-F_0) \right]} + \alpha \frac{\left[2 \left(\frac{\lambda_s}{\lambda_f} \right)^2 \phi + \left(\frac{\lambda_s}{\lambda_f} \right) (3-2\phi) \right]}{\left[(3-\phi) \left(\frac{\lambda_s}{\lambda_f} \right) + \phi \right]} \quad (7.37)$$

where F_0 is a parameter like F above and β represents degree of consolidation.

Verma et al. [39] concluded that the parameter F could be expressed as

$$F = \exp \left[-\psi \left(\frac{\lambda_f}{\lambda_s} \right)^{1/3} \right] \quad (7.38)$$

Here ψ is the sphericity of the particles. The value of F given by Verma et al. is 0.82 for granular systems and 0.75 for emulsion-like systems. They have also applied a resistor model to obtain the expression for λ_e of a two-phase system with spherical inclusions:

$$\lambda_e = \frac{[\lambda_f \{2.598\phi^{1/3}(\lambda_s - \lambda_f) + 3.224\phi^{-1/3}\lambda_f\}]}{[(1-1.2407\phi^{1/3})\{2.5985\phi^{1/3}(\lambda_s - \lambda_f) + 3.224\phi^{-1/3}\lambda_f\} + \lambda_f]} \quad (7.39)$$

where ϕ is the volume fraction of the solid phase.

Misra et al. [40] improved this relation by replacing ϕ by porosity correction term F_p and provided a relation for λ_e as

$$\lambda_e = \frac{[\lambda_f \{2.598F_p^{1/3}(\lambda_s - \lambda_f) + 3.224F_p^{-1/3}\lambda_f\}]}{[(1-1.2407F_p^{1/3})\{2.5985F_p^{1/3}(\lambda_s - \lambda_f) + 3.224F_p^{-1/3}\lambda_f\} + \lambda_f]} \quad (7.40)$$

where $F_p = \exp[-C_2(1-\phi)^{2/3}]$. The value of constant C_2 can be further expressed as

$$C_2 = 2.736e^{-0.004(\lambda_s/\lambda_f)}$$

Singh et al. [41] presented a geometrical model for estimation of the effective thermal conductivity by using the resistors approach of two-phase systems with spherical inclusions. Their expressions for spherical and cubic particles are

$$\lambda_e = \frac{[\lambda_f\{\lambda_f + 0.8060F^{2/3}(\lambda_s - \lambda_f)\}]}{[\lambda_f + F^{2/3}\{0.8060(\lambda_s - \lambda_f)(1 - 1.2407F^{1/3})\}]} \quad (7.41)$$

$$\lambda_e = \frac{[\lambda_f\{\lambda_f + F^{2/3}(\lambda_s - \lambda_f)\}]}{[\lambda_f + F^{2/3}\{(\lambda_s - \lambda_f)(1 - F^{1/3})\}]} \quad (7.42)$$

where F , the porosity correction, is written as

$$F = [1 - \exp\{-0.92\phi_s^2 \ln(\lambda_s/\lambda_f)\}]$$

Recently Moosavi and Sarkomaa [42] presented a theoretical expression for estimating λ_e of three phase composite materials by incorporating circular cylindrical geometry. Their expression is written as

$$\lambda_e = 1 - \frac{2f_1}{(\lambda_1\lambda_2 - \xi_1\xi_2)/(\lambda_2 - \xi_2)} - \frac{2f_2}{(\lambda_1\lambda_2 - \xi_1\xi_2)/(\lambda_1 - \xi_1)} \quad (7.43)$$

where

$$\lambda_i = \frac{1}{\gamma_i} + c_1 f_i - c_2 \gamma_i f_i^4 - c_3 \gamma_{2-\delta_{i2}} f_i f_{2-\delta_{i2}}^3$$

$$\xi_i = c_4 f_i - c_5 (\gamma_i f_i^4 + \gamma_{2-\delta_{i2}} f_i f_{2-\delta_{i2}}^3)$$

$$\gamma_i = \frac{1 - k_i}{1 + k_i}$$

where λ_i is the thermal conductivity of the i th phase, f_i is the volume fraction of the i th phase and c_1 , c_2 , c_3 , c_4 and c_5 are constants.

Boomsma and Poulikakos [43] have developed a model for the effective thermal conductivity of saturated porous metal foams based on three-dimensional geometry for a unit cell termed the tetrakaidecahedron (Figure 7.3). The foam structure was

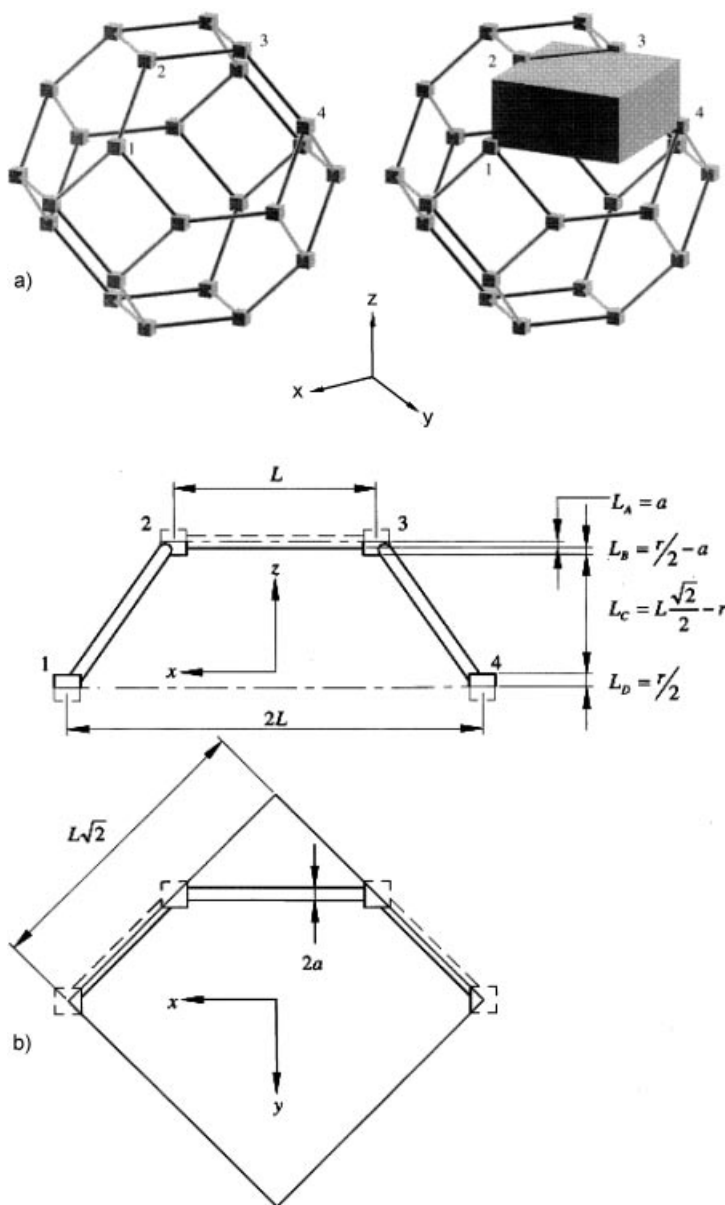


Figure 7.3 (a) The tetrakaidecahedron geometry with cylindrical ligaments and cubic nodes. The unit cell is shown on the right as a solid block located in a single tetrakaidecahedron cell. (b) The geometrical breakdown of the unit cell of the tetrakaidecahedron.

represented with cylindrical ligaments attached to cubical nodes at their centers. The resultant expression for λ_e so obtained is

$$\lambda_e = \frac{\sqrt{2}}{2[R_A + R_B + R_C + R_D]} \quad (7.44)$$

where

$$\begin{aligned} R_A &= \frac{4F}{[2e^2 + \pi F(1-e)\}\lambda_1 + \{4-2e^2-\pi F^2(1-e)\}\lambda_2]} \\ R_B &= \frac{(e-2F)^2}{[(e-2F)e^2\lambda_1 + \{2e-4F-(e-2F)e^2\}\lambda_2]} \\ R_C &= \frac{(\sqrt{2}-2e)^2}{[2\pi F^2(1-2\sqrt{2}e)\lambda_1 + 2\{\sqrt{2}-2e-\pi F^2(1-2\sqrt{2}e)\}\lambda_2]} \\ R_D &= \frac{2e}{[e^2\lambda_1 + (4-e^2)\lambda_2]} \\ F &= \sqrt{\frac{\sqrt{2}\{2-(5/8)e^3\sqrt{2}-2(1-\phi)\}}{(3-4e\sqrt{2}-e)\pi}} \end{aligned}$$

and $e = 0.339$.

Calmidi and Mahajan [44] developed a model for high-porosity fibrous metal foams based on the structure of a metal foam matrix. They assumed that the structure of a metal foam consisted of dodecahedron-like cells with 12–14 hexagonal faces (Figure 7.4). The lumping of material at the point of intersection of the fibers was taken into account as square. The expression for λ_e is written as

$$\begin{aligned} \lambda_e &= \left[\left(\frac{2}{\sqrt{3}} \right) \left\{ \frac{r \left(\frac{b}{L} \right)}{\lambda_f + \left(1 + \frac{b}{L} \right) \frac{(\lambda_s - \lambda_f)}{3}} + \frac{(1-r) \left(\frac{b}{L} \right)}{\lambda_f + \frac{2}{3} \left(\frac{b}{L} \right) (\lambda_s - \lambda_f)} \right. \right. \\ &\quad \left. \left. + \frac{\frac{\sqrt{3}}{2} - \frac{b}{L}}{\lambda_f + \frac{4r}{3\sqrt{3}} \left(\frac{b}{L} \right) (\lambda_s - \lambda_f)} \right\} \right]^{-1} \quad (7.45) \end{aligned}$$

where

$$\frac{b}{L} = \frac{-r + \sqrt{r^2 + \frac{2}{\sqrt{3}}(1-\phi) \left\{ 2 - r \left(1 + \frac{4}{\sqrt{3}} \right) \right\}}}{\frac{2}{3} \left\{ 2 - r \left(1 + \frac{4}{\sqrt{3}} \right) \right\}}$$

Here r is defined as area ratio.

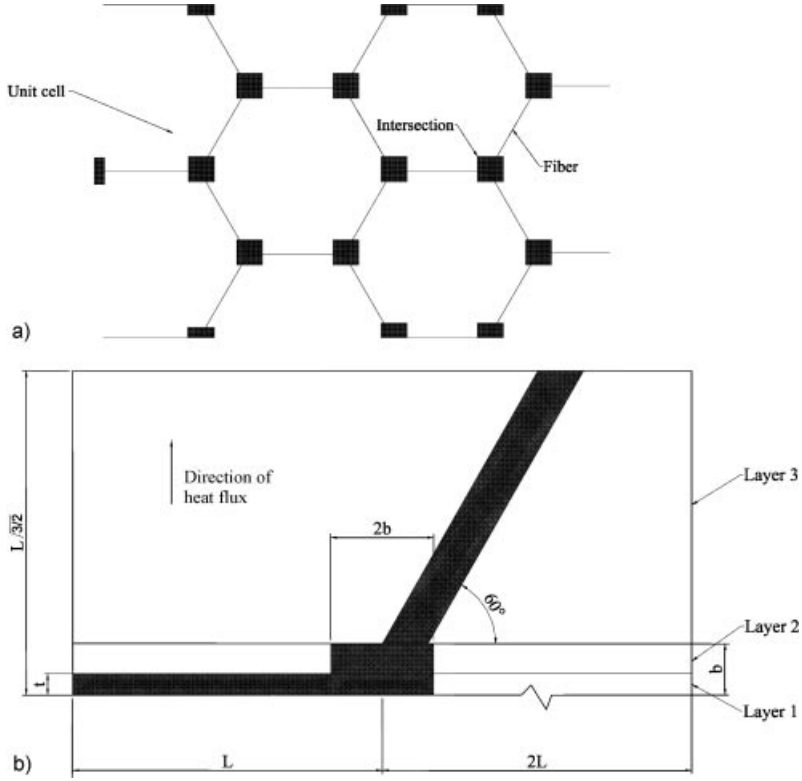


Figure 7.4 (a) Hexagonal structure of metal foam matrix. (b) Unit cell representation of hexagonal structure.

An analytical model was given by Bhattacharya et al. [45] for highly porous metal foams (Figure 7.5). With the hexagonal geometry and two-dimensional array of hexagonal cells, the expression for λ_e is

$$\lambda_e = \left[\left(\frac{2}{\sqrt{3}} \right) \left\{ \frac{\left(\frac{t}{L} \right)}{\lambda_2 + \frac{(\lambda_1 - \lambda_2)}{3}} + \frac{\frac{\sqrt{3}}{2} - \frac{t}{L}}{\lambda_2} \right\} \right]^{-1} \quad (7.46)$$

where

$$\frac{t}{L} = \frac{-\sqrt{3} - \sqrt{3 + (1 - \phi_1)(\sqrt{3} - 5)}}{1 + \frac{1}{\sqrt{3}} - \frac{8}{3}}$$

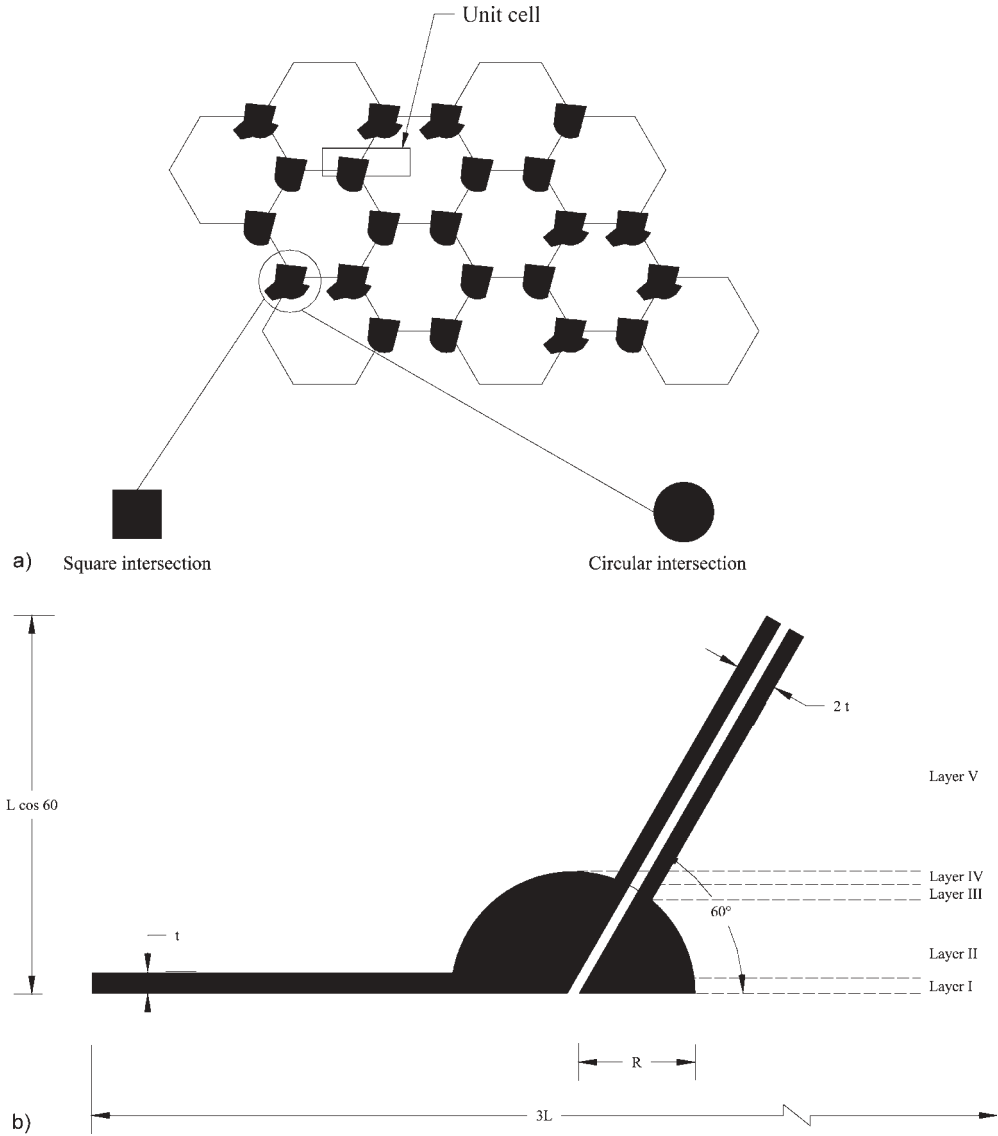


Figure 7.5 (a) Analytical geometry for thermal conductivity.
(b) Unit cell representation for circular intersection.

and

$$\lambda_e = F\{\phi_1\lambda_1 + (1-\phi_1)\lambda_2\} + \frac{(1-F)}{\left\{\frac{\phi_1}{\lambda_1} + \frac{(1-\phi_1)}{\lambda_2}\right\}}$$

where $F = 0.35$.

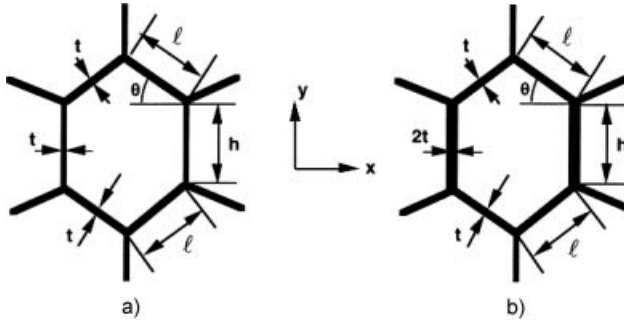


Figure 7.6 Unit cell of a hexagonal honeycomb (a) with uniform thickness cell walls and (b) with nonuniform thickness cell walls.

Lu and Chen [46] presented a theoretical approach by considering a system made of hexagonal honeycombs (Figure 7.6). The conductivities of a hexagonal honeycomb are in general anisotropic and can be represented by a second-order tensor. The resulting conductivities expressed in the (x, y, z) directions are

$$\begin{aligned}\lambda_x &= \rho \lambda_s \frac{\cos^2 \theta}{(1 + h/l)} \\ \lambda_y &= \rho \lambda_s \left(\frac{h/l + \sin \theta}{1 + h/l} \right)^2 \\ \lambda_z &= \rho \lambda_s\end{aligned}\tag{7.47}$$

where

$$\rho = \frac{(1 + h/l)t/l}{\cos \theta (h/l + \sin \theta)}$$

Recently Singh and Kasana [19] developed an empirical relation or quick estimation of effective thermal conductivity of highly porous systems. In order to incorporate varying individual geometries and nonlinear flow of heat flux lines generated by the difference in thermal conductivity of the constituent phases, a correlation term has been introduced. The expression is

$$\lambda_e = \lambda_{||}^F \cdot \lambda_{\perp}^{(1-F)} \quad F \geq 0, \quad 0 \leq F \leq 1\tag{7.48}$$

where $\lambda_{||} = \phi \lambda_f + (1 - \phi) \lambda_s$ and

$$\lambda_{\perp} = \frac{\lambda_s \lambda_f}{(1 - \phi) \lambda_f + \phi \lambda_s}$$

are upper and lower bounds on the effective thermal conductivity respectively and F is given by

$$F = C \left\{ 0.3031 + 0.0623 \ln \left(\phi \frac{\lambda_s}{\lambda_f} \right) \right\}$$

where C is a numerical constant that depends on the nature of the material.

Jaggiwanram and Singh [47] generalized Singh's model assuming inclined slabs with the heat flux lines and derived a relation as

$$\lambda_e = \left[(\phi \lambda_s + (1-\phi) \lambda_f)^2 \cos^2 \theta + \frac{\lambda_s^2 \lambda_f^2 \sin^2 \theta}{(\phi \lambda_f + (1-\phi) \lambda_s)^2} \right]^{1/2} \quad (7.49)$$

where $\sin^2 \theta = C_1 \phi^{1/2} \ln(\lambda_s/\lambda_f) + C_2$ and constants C_1 and C_2 are different for each type of material.

7.2.2

Discussion

We have briefly reviewed various existing models used for predicting λ_e . A number of different geometries like plates, cubes, spheres, ellipsoids and hexagons arranged in a particular order were considered. The real structures and geometries of materials around us are so vast and varied, that one cannot use a single expression to explain thermal conduction in various systems. In real systems, the kind of geometry we face does not match with the geometries discussed in the literature. Therefore results of these models vary with the experimental results. Particularly in two-phase systems the deviation of results depends on the ratio of thermal conductivities of solid and fluid phase. Another parameter affecting the result is the density of the dispersed phase.

Most of the models discussed in this section are developed either using the concept of modified flux or considering the phases made of different resistors. The resistor concept embodies linear flow of heat where Ohm's law is followed, while the flux concept is based on material field from external or internal sources and thus the flux density and its path depends upon the conductivity of the material through which the heat flow is maintained. These models do not describe the behavior of an actual system. The resistor model is an exact solution for a two-phase system arranged in the form of slabs while the flux model is an exact solution whose micro-geometry and phase distribution is completely prescribed like spheres in a cubic array with lattice-type structures. In general, the materials around us do not belong to either category as their phase distribution and grain arrangement is completely undefined. Therefore, the models developed using these concepts cannot be directly applied to natural two-phase materials. However, at the same time, the resistor model yields the maximum and minimum limits on λ_e . Similarly, the flux model gives an insight as to how the flux modification takes place in a periodic structure like beads which are statistically homogeneous but locally heterogeneous.

The difference between real and assumed situations increases rapidly as the ratio of component conductivity increases or decreases from a moderate value. This led to a new idea, i.e. randomization of phase distribution. The resulting expression for λ_e depends upon the method of randomization applied.

The idea of random phase distribution using the flux concept resulted in Maxwell's relation, Fricke's relation, the Bruggeman theory of variable dispersion and the relation of Brailsford and Major. The relation established by Maxwell is suitable for dilute dispersion and moderate conductivity ratios. The results of Maxwell's formula are satisfactory for $\phi = 0.5$. The concept of randomization used in resistor models with averaging techniques is better reflected in models of Woodside and Messmer, Chaudhary and Bhandari, Kumar and Chaudhary and Cheng and Vachon.

The model developed by Lichtnecker does not incorporate structure and mode of packing of a system. It is suitable at very low and very high dispersions. When the ratio of thermal conductivities of solid and fluid phase is more than 20, the value predicted for λ_e is overestimated. The expression of Rayleigh is restricted to cellular materials and emulsions. The relation of Fricke and Burgers gives a good result for packed systems of quartz sand and glass beads in different fluids only. The expression of Kunni and Smith provides a lower value of λ_e for lower ratio of thermal conductivities of solid and fluid phase. Sugawara and Yoshizawa provided an empirical relation for λ_e , which yields correct values of λ_e for soils. They used $n = 6.5$ in their equation (Eq. 7.21).

The bound technique is really useful in estimating the closest optimum value of λ_e of two-phase systems. The Hashin–Strikman bound is a most general bound which predicts λ_e with the least possible knowledge about the two-phase system. The Hashin–Strikman bound is of wider use in the range $0.1 < \lambda_d/\lambda_c < 10$. Moreover, when the ratio (λ_d/λ_c) becomes too large or too small, the Hashin–Strikman bound becomes broader and turns out to be unrealistic. The Kumar and Chaudhary bound is equally well in the region $0.1 < \lambda_d/\lambda_c < 10$ but at the same time it is narrower than the Hashin–Strikman bound when $\lambda_d/\lambda_c < 10^{-2}$ in the case of sands and soils.

The expressions developed on the basis of an averaging technique seem to be more relevant than the models, which are the outcome of rigorous mathematics. As an example, the results of Hadley's model are better than those of Lichtnecker, Brailsford and Pande. Pande's model is better when the fluid phase is air in a two-phase system. The model developed by Boomsma and Poulikakos is based on the idealized three-dimensional basic cell geometry of foam, the tetrakaidecahedron. This geometric shape results from filling a given space with cells of equal size yielding minimal surface energy. The foam structure was represented with cylindrical ligaments, which attach to cubic nodes at their centers. It was found that the model estimated the effective thermal conductivity very well for these experimental configurations. This three-dimensional model fits the experimental data very well for the parameter range experienced in metal foams. Bhattacharya et al. in their model considered that the structure consists of a two-dimensional array of hexagonal cells where the fibers form the sides of the hexagons and a circular blob of the metal at the intersection of the fibers. Their analysis reflected that λ_e depends strongly on the porosity and the ratio of the cross-sections of the fiber and intersection.

Now, there is a trend to develop models using numerical simulations including some unknown parameters. The value of these parameters is found to vary according to situations arising due to the applicability of the material. Models developed using these techniques are not discussed here because of the limitations of space.

7.3

Experimental Techniques

The techniques of measuring thermal conductivity can be divided into two categories, steady state and dynamical, depending on the temperature distribution with time. Steady-state techniques used to measure the effective thermal conductivity demand careful experimentation to minimize heat losses. An establishment of steady state in large mass is a slow and time-consuming process. It is this reason which prompted many researchers to explore the possibility of employing dynamic techniques. Dynamical methods can also be divided into two categories, periodic or transitory, depending on whether the thermal energy is supplied to the sample is in the form of a pulse for a fixed period or as a constant power. As a consequence, the change in temperature in the sample is periodic or transient.

The main differences among these techniques are the shape of the heating elements and their ability to cover as large as possible a range of transport properties with satisfactory accuracy. In these techniques, a resistive element is used as the heat source and often also as a temperature sensor. In order to provide applicability for small samples and high-sensitivity temperature measurements the element should be thin and the resistance as large as possible. However, it may be noted that while using these devices the geometrical configuration of the heating element and contact resistance are very important parameters. One of the important aspects of these methods is that by using a very short time scale in the measurements, it becomes possible to approximate closely the mathematical description of the temperature distribution around the heating element. Because of the short heating time there is an appreciable increase in temperature in the immediate neighborhood of the heating element only. There is a growing need across for rapid, compact and preferably *in situ* devices for measurement of thermophysical properties. In view of these, it is more convenient to use nonsteady-state techniques for the measurement of thermal conductivity. However, the choice of a particular technique depends upon the type of material under investigation. In the following sections (Sections 7.3.1–7.3.5) we discuss some of the important experimental techniques commonly used for measurement of the thermal conductivity of porous materials.

7.3.1

Thermal Conductivity Probe

Thermal conductivity probes have been widely used for determination of thermal conductivity of liquids and porous and granular materials. Many researchers have used the line heat source technique for several years for measuring the effective

thermal conductivity of liquids, solids, loose granular materials, metallic powders and dispersed systems. Several authors [48–50] used this technique for the determination of thermal conductivity of soils. Due to the simplicity of this technique and the low cost of instrumentation, the probe method has been frequently used for the determination of the effective thermal conductivity. Vander Held and Van Drunen [51] have used the probe method for determination of the effective thermal conductivity of liquids.

The thermal probe is essentially a metallic needle consisting of constant power heater and thermocouple as temperature sensor (Figure 7.7). This method is obtained from the theory of heat conduction from a buried heat source in an infinite homogeneous medium. The rate of heat dissipation in the material is a function of thermal conductivity apart from other parameters. An important feature of the thermal probe is that one can estimate temperature distribution

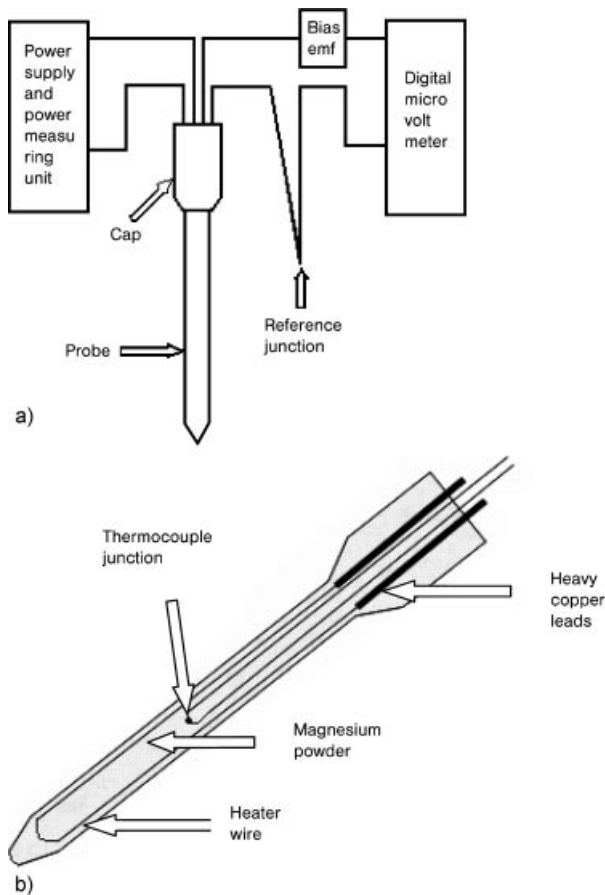


Figure 7.7 (a) Experimental setup for determination of thermal conductivity.
(b) Thermal conductivity probe.

around the heating element in a short duration of time. In the following a brief discussion of the theory of the thermal conductivity probe is given.

7.3.1.1 Theory

When a line source of heat is buried in an infinite homogeneous medium, the temperature rise with respect to time at a point near to the line source depends on the rate of heat transfer and various thermophysical properties of the surroundings. The temperature rise T can be expressed by the following expression [52]:

$$T = \frac{q}{2\pi\lambda} \int_{r\xi}^{\infty} \frac{e^{-\beta^2}}{\beta} d\beta = \frac{q}{2\pi\lambda} I(r\xi) \quad (7.50)$$

where

$$\xi = \frac{1}{\sqrt{4\kappa t}}, \quad \beta = \frac{t'}{2\sqrt{\kappa(t-t')}}$$

and

$$I(r\xi) = \gamma - \ln(r\xi) + \frac{1}{2}(r\xi)^2 - \frac{1}{8}(r\xi)^4 + \frac{1}{36}(r\xi)^6 \dots$$

λ = thermal conductivity of the sample, κ = thermal diffusivity of the sample, γ = Euler's constant having value 0.5772, q = rate of heat generation in the line source per unit length and per unit time, r = distance of any point inside the sample from the line source and t = time from start of the heating. Therefore, Eq. (7.50) can be written as

$$T = \frac{q}{4\pi\lambda} \left[-\gamma + \ln\left(\frac{4\kappa t}{r^2}\right) + \frac{r^2}{4\kappa t} - \frac{1}{4} \frac{r^4}{(4\kappa t)^2} + \frac{1}{18} \frac{r^6}{(4\kappa t)^3} - \dots \right] \quad (7.51)$$

When $r^2 \ll 4\kappa t$, then the above equation reduces to

$$T = \frac{q}{2\pi\lambda} \left[\gamma - \ln\left(\frac{r}{\sqrt{4\kappa t}}\right) \right] \quad (7.52)$$

If the temperature at a certain point can be measured at two different times t_1 and t_2 , then the effective thermal conductivity measured by probe method can be expressed as

$$\lambda = \frac{q}{4\pi} \frac{\ln(t_2/t_1)}{(T_2 - T_1)} \quad (7.53)$$

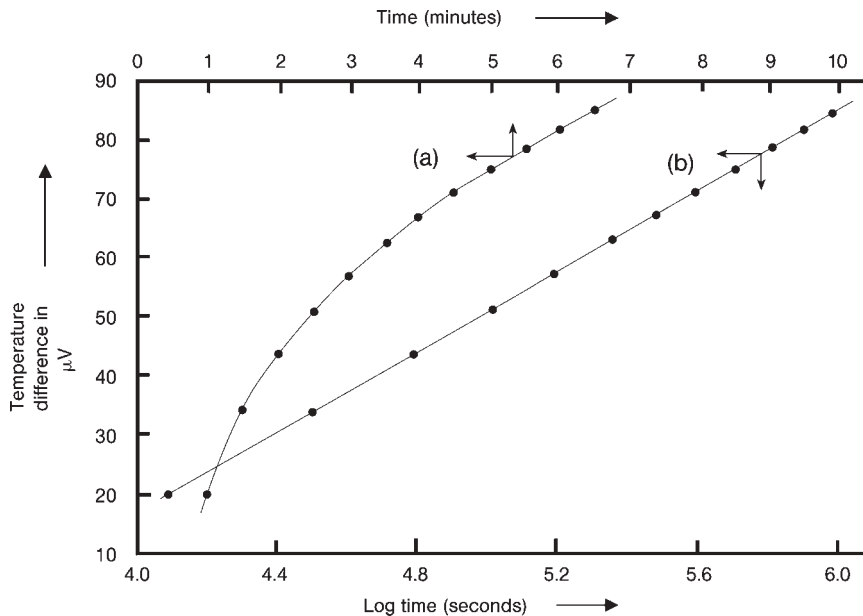


Figure 7.8 Probe temperature time profiles: (a) temperature versus time; (b) temperature versus logarithm of time.

If the length of the probe is L , the resistance of the heater wire of the probe is R and current passing through the heater wire is I , then power per unit length will be $q = I^2 R/L$.

Therefore, the expression for effective thermal conductivity can be written as

$$\lambda = \frac{I^2 R \ln(t_2/t_1)}{4\pi L (T_2 - T_1)} \quad (7.54)$$

By using Eq. (7.54), the effective thermal conductivity can be determined experimentally.

The theory of the transient method for thermal conductivity has been given by Hsu [53]. A line heat source should not occupy any space and should be massless theoretically. Practically the line heat source consists of a fine heater wire housed in a hollow cylindrical needle, which has a finite radius. The thermal characteristics of this line source also differ from the material in consideration. Vander Held and Drunen [51] and De Vries and Peck [54] have analyzed these practical discrepancies in detail (Figure 7.8).

7.3.2

Differential Temperature Sensor Technique

In this technique, the parallel wire method has been modified [55]. Two thermocouples at different distances are mounted parallel to the needle (Figure 7.9). This

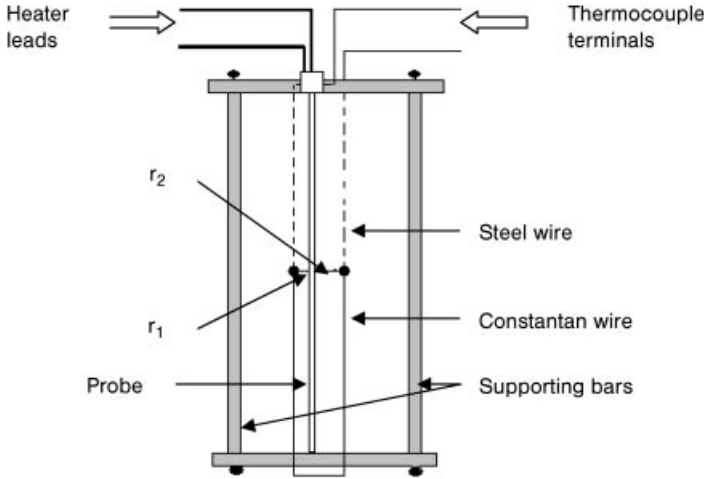


Figure 7.9 Differential temperature sensor probe.

modification not only improves the performance of the transient probe, but also makes it a device for simultaneous determination of all the thermophysical parameters.

7.3.2.1 Mathematical Analysis

If the rise in temperature at two near points, distant r_1 and r_2 , be T_1 and T_2 , respectively, then from the theory of line heat source (Eq. 7.51) we have

$$T_1 = \frac{q}{4\pi\lambda} \left[-\gamma + \ln\left(\frac{4\kappa t}{r_1^2}\right) + \frac{r_1^2}{(4\kappa t)} - \frac{1}{4} \frac{r_1^4}{(4\kappa t)^2} + \cdots \frac{2\lambda}{bH} \right] \quad (7.55)$$

and

$$T_2 = \frac{q}{4\pi\lambda} \left[-\gamma + \ln\left(\frac{4\kappa t}{r_2^2}\right) + \frac{r_2^2}{(4\kappa t)} - \frac{1}{4} \frac{r_2^4}{(4\kappa t)^2} + \cdots \frac{2\lambda}{bH} \right] \quad (7.56)$$

where $2\lambda/bH$ is called the initial lag error and arises due to the thermal mass of the probe and contact resistance between the probe and the sample. Here b and H are the probe radius and the contact conductance at the probe medium interface. Subtracting these two, we get

$$T_1 - T_2 = \frac{q}{4\pi\lambda} \left[\ln\left(\frac{4\kappa t}{r_1^2}\right) - \ln\left(\frac{4\kappa t}{r_2^2}\right) - \frac{r_2^2 - r_1^2}{(4\kappa t)} + \frac{1}{4} \frac{r_2^4 - r_1^4}{(4\kappa t)^2} \right] \quad (7.57)$$

To account for time lag, the correction term t_c has to be subtracted from the observed time. As $t \gg t_c$, the above equation may be written as

$$T_1 - T_2 = \frac{q}{4\pi\lambda} \left[\ln\left(\frac{r_2}{r_1}\right)^2 - \frac{r_2^2 - r_1^2}{(4\kappa)} \frac{1}{t} + \frac{r_2^2 - r_1^2}{(4\kappa)} \left(\frac{r_2^2 + r_1^2}{(16\kappa)} - t_c \right) \frac{1}{t^2} \right] \quad (7.58)$$

Here we have retained terms up to second power in $(1/t)$. The equation between $(T_1 - T_2)$ and $(1/t)$ represents a parabola of the form

$$\gamma = B_0 + B_1 x + B_2 x^2 \quad (7.59)$$

Knowing the values of these constants (B_0 , B_1 , B_2) the thermal conductivity and thermal diffusivity can be determined by the following relations:

$$\lambda = \frac{q}{2\pi B_0} \ln\left(\frac{r_2}{r_1}\right) \quad (7.60)$$

$$\kappa = \frac{1}{8} \frac{B_0}{B_1} \frac{(r_2^2 - r_1^2)}{\ln\left(\frac{r_2}{r_1}\right)} \quad (7.61)$$

While evaluating Eqs. (7.60) and (7.61), one has to depend on calculations for λ and κ by plotting a graph

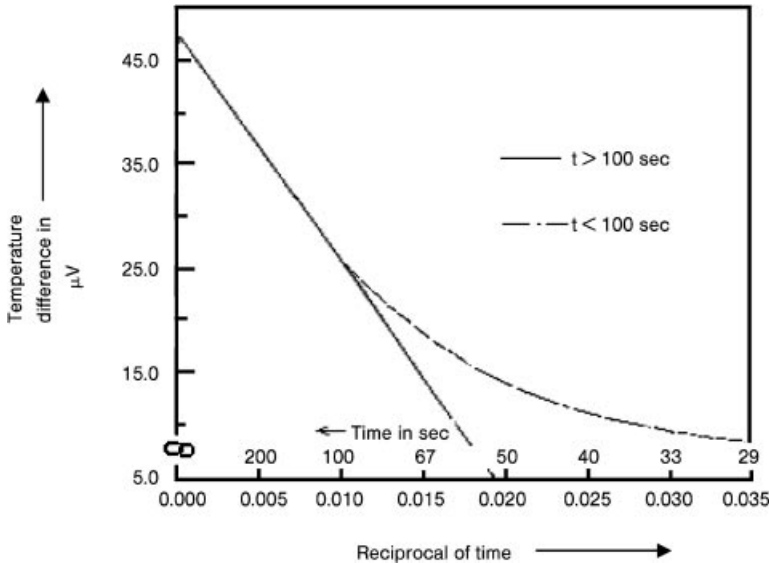


Figure 7.10 Temperature–time profiles for a differential temperature sensor probe.

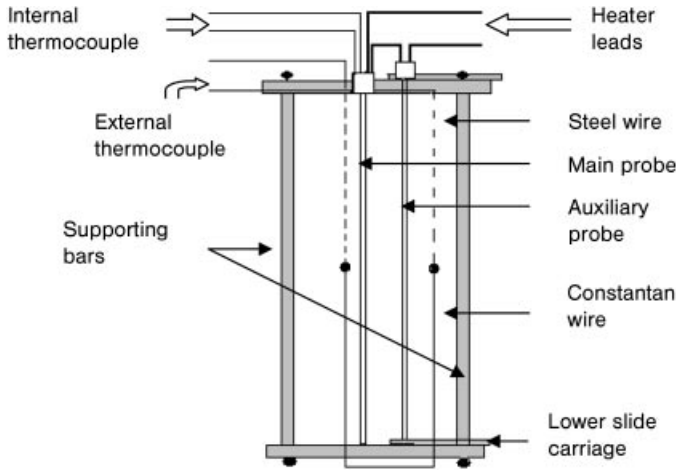


Figure 7.11 Probe-controlled transient device.

7.3.3

Probe-Controlled Transient Technique

Higher order terms in Eq. (7.51) can also be made insignificant in an ingenious way by mounting a low-power auxiliary probe on the parallel wire assembly as shown in Figure 7.11. This probe may be mounted on a light carriage which can slide on the assembly itself [56]. It has its own temperature sensor in the form of a thermocouple which is connected to the thermocouple of the main probe. Thus the thermo e.m.f. generated by it will be in the opposite direction to the one produced by the main probe. By doing this, the thermo e.m.f. generated by the main probe can be modified. Therefore, the thermo e.m.f. produced by the assembly can be controlled in a desired manner by varying the position of the auxiliary probe with respect to its sensor. This device can be used with constant power method and with pulse method. When used with the pulse technique it accurately determines both the thermal conductivity and thermal diffusivity.

7.3.3.1 Mathematical Analysis

Constant Power Method Neglecting the third and higher powers of $(1/t)$ in Eq. (7.51) and taking the lag correction term into account the difference in temperature will be

$$T_1 - T_2 = \frac{I^2}{4\pi\lambda L} \left[-\gamma(R_1 - R_2) + (R_1 - R_2) \ln(4\kappa t) + \ln \left(\frac{r_2^{2R_2}}{r_1^{2R_1}} \right) + \frac{R_1 r_1^2 - R_2 r_2^2}{4\kappa t} - \frac{R_1 r_1^4 - R_2 r_2^4}{4(4\kappa t)^2} + \dots \frac{2\lambda}{bH} (R_1 - R_2) \right] \quad (7.62)$$

where R_1 and R_2 are the resistances of first and second probes respectively and L is the length of both the probes. As the heaters of the two probes are connected in series, so the same current I will flow through both the probes. Here in Figure 7.11, the two thermocouples are connected in subtractive mode.

If $R_1 r_1^2 - R_2 r_2^2 = 0$, then

$$T_1 - T_2 = \frac{I^2}{4\pi\lambda L} \left[-\gamma(R_1 - R_2) + (R_1 - R_2)\ln(4\kappa t) + \ln\left(\frac{r_2^2 R_2}{r_1^2 R_1}\right) + \dots \frac{2\lambda}{bH}(R_1 - R_2) \right]$$

The term containing $(1/t)$ disappears as the numerator is zero, whereas the term containing $(1/t^2)$ can be neglected because the denominator increases rapidly. Hence the above expression can also be written as

$$T_1 - T_2 = \frac{I^2 C}{4\pi\lambda L} + \frac{I^2(R_1 - R_2)}{4\pi\lambda L} \ln(t) \quad (7.63)$$

where

$$C = \left[-\gamma(R_1 - R_2) + (R_1 - R_2)\ln(4\kappa) + \ln\left(\frac{r_2^2 R_2}{r_1^2 R_1}\right) + \dots \frac{2\lambda}{bH}(R_1 - R_2) \right]$$

Equation (7.63) shows that the plot $(T_1 - T_2)$ versus $\ln(t)$ will be a straight line having a slope C' . Therefore, the thermal conductivity of the medium can be determined by the relation

$$\lambda = \frac{I^2(R_1 - R_2)}{4\pi C' L} \quad (7.64)$$

Pulse Method If a pulse of power $q = I^2 R \tau / L$ is passed through the probe, then the rise in temperature at a near point is given by the expression [58]

$$T = \frac{I^2 R \tau}{4\pi\lambda L} \left[\frac{1}{t} e^{-\frac{r^2}{4\kappa t}} \right] \quad (7.65)$$

where τ is the duration of the pulse. If the lag correction is taken into account the rise in temperature due to the first probe will be

$$T_1 = \frac{I^2 R_1 \tau}{4\pi\lambda L} \left[\frac{1}{t} e^{-\frac{r_1^2}{4\kappa t}} + \frac{2\lambda}{bH} \right] \quad (7.66)$$

And the rise in temperature due to the second probe will be

$$T_2 = \frac{I^2 R_2 \tau}{4\pi\lambda L} \left[\frac{1}{t} e^{-\frac{r_2^2}{4\kappa t}} + \frac{2\lambda}{bH} \right] \quad (7.67)$$

As the thermocouples are in subtractive mode, net rise in temperature will be

$$T_1 - T_2 = \frac{I^2 \tau}{4\pi\lambda L} \left[\frac{R_1}{t} e^{-\frac{r_1^2}{4\kappa t}} - \frac{R_2}{t} e^{-\frac{r_2^2}{4\kappa t}} + \frac{2\lambda(R_1 - R_2)}{bH} \right] \quad (7.68)$$

Expanding it into powers of $(1/t)$ and if $(r_1^4 R_1 - r_2^4 R_2) = 0$, then we have

$$T_1 - T_2 = \frac{I^2 \tau}{4\pi\lambda L} \left[(R_1 - R_2) \frac{1}{t} - \frac{r_1^2 R_1 - r_2^2 R_2}{4\kappa} \frac{1}{t^2} - \frac{r_1^6 R_1 - r_2^6 R_2}{6(4\kappa)^3} \frac{1}{t^4} \dots + \frac{2\lambda(R_1 - R_2)}{bH} \right] \quad (7.69)$$

The term containing $(1/t^3)$ becomes zero and that containing $(1/t^4)$ becomes negligible by virtue of the time being large and numerator being small. Hence the net rise in temperature can be written as

$$T_1 - T_2 = B_0 + B_1 \frac{1}{t} - B_2 \frac{1}{t^2} \quad (7.70)$$

where

$$B_0 = \frac{I^2 (R_1 - R_2) \tau}{2\pi bHL}$$

$$B_1 = \frac{I^2 (R_1 - R_2) \tau}{4\pi\lambda L}$$

$$B_2 = \frac{I^2 \tau (r_1^2 R_1 - r_2^2 R_2)}{4\pi\lambda L (4\kappa)}$$

Therefore,

$$\lambda = \frac{I^2 (R_1 - R_2) \tau}{4\pi L B_1} \quad (7.71)$$

and

$$\kappa = \frac{1}{4} \frac{B_1 (r_1^2 R_1 - r_2^2 R_2)}{B_2 (R_1 - R_2)} \quad (7.72)$$

The behavior of the device can be controlled by varying r_2 , the distance of the auxiliary probe with respect to its sensor. By selecting a proper value of r_2 , the undesired term of the series can be eliminated. Therefore, the sensitivity of the instrument can be controlled in a desired manner.

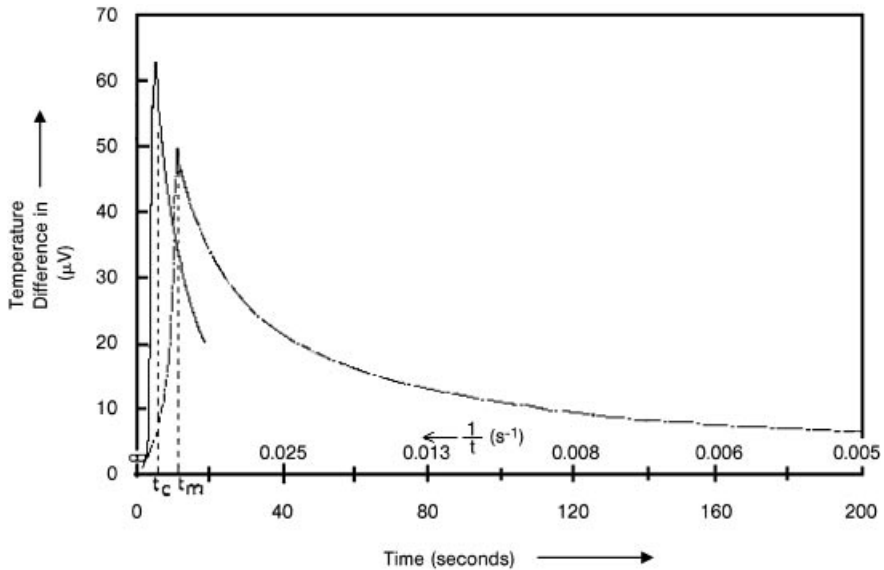


Figure 7.12 Temperature–time profiles for a probe-controlled transient device with pulse technique.

7.3.4

Plane Heat Source

The heat storage coefficient is an important thermophysical parameter, which can very well explain the thermal behavior of a system and its applications. This parameter characterizes a medium on the basis of its heat storage ability. When heat is provided to a medium, then some of it is retained by the first section of the medium and the rest is transferred to the subsequent layers of the medium. While at steady state all the heat is transferred to subsequent layers. At nonsteady state, heat retained by a particular layer is a function of its heat storage coefficient. In this section, we describe the measurement technique of the heat storage coefficient for different kinds of materials (Figures 7.13 and 7.14). This method of measurement is named the “plane heat source” technique [57].

7.3.4.1 Theory

Consider a plane heat source located at a distance $x = u$ in an infinite medium. This source generates q units of heat per unit area flowing along the x direction. Heat conduction in such a medium is represented as [58]

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\kappa} \frac{\partial T}{\partial t} \quad (7.73)$$

where κ is the thermal diffusivity of the system. At $t = 0$, $T = f(x)$.

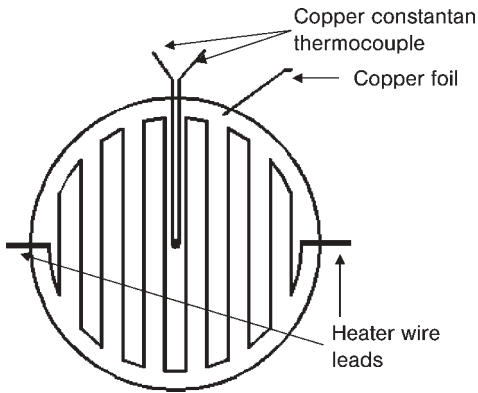


Figure 7.13 Design of plane heat source.

When the heat generated penetrates into the medium, the temperature of unit area of medium between planes u and $u + du$ increases as

$$\frac{q'}{\rho c \Delta u} = \frac{S}{\Delta u}$$

where ρ and c are the density and specific heat of the medium, respectively, and S is termed the strength of the source. The rise in temperature T at any point x in the

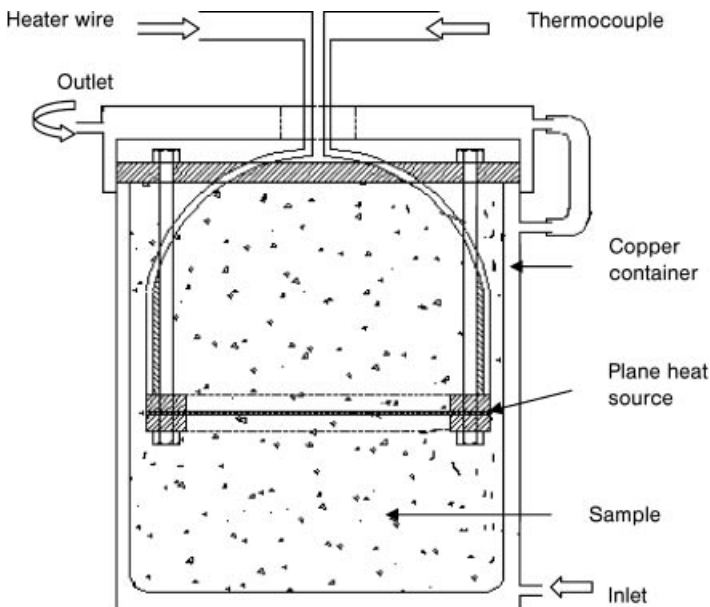


Figure 7.14 Experimental setup for the measurement of β_e .

medium is represented as [59]

$$T = \frac{S\eta}{\Delta u \sqrt{\pi}} \int_u^{u+du} \exp[-(u-x)\eta^2] du \quad (7.74)$$

Here $\eta = 1/\sqrt{4\kappa t}$ and $f(u) = 0$ outside the limit of integration. Let us consider that the mean value of $\exp[-(u-x)\eta^2]$ between the above limits of integration is $\exp[-(u'-x)\eta^2]$ under the condition that $u < u' < (u + du)$. Thus

$$T = \frac{S\eta}{\sqrt{\pi}} \exp[-(u'-x)\eta^2] \quad (7.75)$$

When $\Delta u \rightarrow 0$,

$$T = \frac{S\eta}{\sqrt{\pi}} \exp[-(u-x)\eta^2] \quad (7.76)$$

Let us take a fixed source S' at $x = u$ providing a constant output heat at time $t = 0$. We can obtain the temperature distribution due to this source at any time t by taking the summation of each effect of S that has occurred at a time $(t - \tau)$ earlier. Here τ represents time variable in the limits from 0 to t . The increment in time can be calculated by replacing S by $S' \cdot d\tau$ and t by $(t - \tau)$ in Eq. (7.76) and finally integrating it in the limits provided. If we include the position of the source at the origin, then Eq. (7.76) will result in

$$T = \frac{S'}{2\sqrt{\pi\kappa}} \int_0^t \exp\left[-\left\{\frac{x^2}{4\kappa(t-\tau)}\right\}\right] (t-\tau)^{-1/2} d\tau \quad (7.77)$$

Substituting

$$b = \frac{x}{2\sqrt{\kappa(t-\tau)}}$$

and

$$S' = \frac{q}{\rho c} = \frac{q\kappa}{\lambda}$$

Eq. (7.77) reduces to

$$T = \frac{S}{2\kappa\sqrt{\pi}} \int_{x^2/2\sqrt{\kappa t}}^{\infty} \frac{\exp(-b^2)}{b^2} db$$

or

$$T = \frac{qx}{2\lambda\sqrt{\pi}} \int_{x\eta}^{\infty} \frac{\exp(-b^2)}{b^2} db \quad (7.78)$$

This equation can be further simplified as

$$T = \frac{qx}{2\lambda} \left[\frac{\exp(-x^2\eta^2)}{x\eta\sqrt{\pi}} - \frac{2}{\sqrt{\pi}} \int_{x\eta}^{\infty} \exp(-b^2) db \right] \quad (7.79)$$

where q denotes the power generated per unit area by the source. For $x=0$,

$$\exp(-x^2\eta^2) = 1 \quad (7.80)$$

and

$$\int_{x\eta}^{\infty} \exp(-b^2) db = 1 \quad (7.81)$$

Therefore for $x=0$, Eq. (7.79) yields

$$T = \frac{q}{2\lambda\eta\sqrt{\pi}} \quad (7.82)$$

By substituting the value of $\eta = 1/\sqrt{4\kappa t}$, we find

$$T = \frac{q\sqrt{\kappa}}{\lambda} \sqrt{\frac{t}{\pi}} \quad (7.83)$$

Further

$$T = \frac{q}{\beta_e} \sqrt{\frac{t}{\pi}} \quad (7.84)$$

where β_e defines the effective heat storage coefficient.

The above equation indicates that the rise in temperature at the center of the source will be proportional to the square root of time. The curve between T and $\sqrt{t}$ will be a straight line. Thus by knowing the required parameters in the above equation, the heat storage coefficient can be determined.

The following points must be taken care of during the fabrication of a plane heat source:

- The requirement of power for the source has been taken to be very low. The mathematical expression for power P_s is given by

$$P_s = V\rho_s c_s \left(\frac{\Delta T}{\Delta t} \right) \quad (7.85)$$

where V = volume of the source, ρ_s = mean density, c_s = mean specific heat, ΔT = rise in temperature and Δt = time of measurements.

- To minimize the lateral heat loss, the thickness of the source is kept as small as possible.
- The property of insulating materials used for the fabrication of plane heat source has to be of top priority. The total observation time is taken least possible to avoid the deviations from the axial heat flow. Initially the self-heating of the source may cause variations in the results.

7.3.5

Transient Plane Source (TPS)

Gustaffsson [60] developed the transient plane source (TPS) technique in which the conducting pattern has a total electrical resistance that is higher and more sensitive than the hot strip or thermal conductivity probe (Figure 7.15). The TPS is a commercial compact instrument commonly using a $10\text{ }\mu\text{m}$ thick nickel double spiral sensor. The sensor has a $25\text{ }\mu\text{m}$ thick layer of Kapton insulation to keep it electrically isolated from the material. The sensor can be used over a temperature range $10\text{--}500\text{ K}$ with Kapton insulation, while for temperatures up to 1000 K , a layer (0.01 mm) of mica insulation is recommended [60].

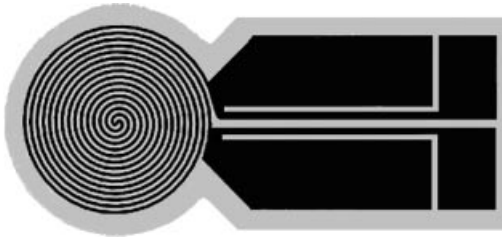


Figure 7.15 Transient plane source sensor.

7.3.5.1 Theory

Two specimens of the same material are brought into contact with the flat sides of a TPS sensor. A constant current is supplied to the sensor. As the sensor temperature

changes, the resistance of the sensor will also change and by recording the resistance of the sensor $\Delta T(\tau)$ can be calculated using the relation

$$\Delta T(\tau) = \frac{1}{\alpha} \left(\frac{R(t)}{R_0} - 1 \right) \quad (7.86)$$

where R_0 is the initial resistance of the sensor and

$$\tau = (t/\theta)^{1/2}, \quad \theta = a^2/\kappa \quad (7.87)$$

Here t is the measurement time and θ is the characteristic time. The constants a and κ are the radius of the sensor and thermal diffusivity of the sample, respectively, and α is the temperature coefficient of the resistance. Since this model assumes the sample to be infinitely large, it is important to be aware of the influence of the specimen boundary using the TPS technique. The probing depth, ΔP , is the thickness of the specimen and helps to determine the minimum size and the transient recording time required to approximate the infinite specimen required by the theory. This is defined as

$$\Delta P = \beta(K \times t_{\max})^{1/2} \quad (7.88)$$

where β is a constant of the order of unity and $t_{\max}$ is the total time of the transient recording.

Assuming the conductive pattern in the Y - Z plane of a coordinate system, the rise in temperature at a point (y, z) at time t due to an output power per unit area Q is given as [60]

$$\Delta T(y, z, t) = \left(8\pi^{\frac{3}{2}} \rho c \right)^{-1} \int_0^t dt' [\kappa(t-t')]^{-\frac{3}{2}} \int_A dy' dz' Q(y', z', t') \exp\{ -[(y-y')^2 + (z-z')^2][4\kappa(t-t')]^{-1} \} \quad (7.89)$$

where ρ , c , and κ are the density, the specific heat and the thermal diffusivity of the material, respectively.

Expression (7.89) is simplified by taking $\kappa(t-t') = \sigma^2 a^2$ as

$$\Delta T(y, z, t) = \left(4\pi^{\frac{3}{2}} a \lambda \right)^{-1} \int_0^{\tau} \frac{d\sigma}{\sigma^2} \int_A dy' dz' \times Q(y', z', t') \exp\left\{ -\frac{[(y-y') + (z-z')]}{4\sigma^2 a^2} \right\} \quad (7.90)$$

The exact solution of Eq. (7.90) is possible in the case of disk geometry [60]. The average increase in temperature of the disk is

$$\Delta T(\tau) = \frac{P_0}{\pi^{3/2} a \lambda} D(\tau) \quad (7.91)$$

where P_0 is the total output power, λ is the thermal conductivity of the material and $D(\tau)$ is a dimensionless function defined as

$$D(\tau) = [m(m+1)]^{-2} \times \int_0^\tau \frac{d\sigma}{\sigma^2} \left[\sum_{l=1}^m l \left\{ \sum_{k=1}^m k \cdot \exp\left(\frac{(-l^2 + k^2)}{2\sigma^2 m^2}\right) L_0\left(\frac{lk}{2\sigma^2 m^2}\right) \right\} \right] \quad (7.92)$$

Here m and L_0 are the number of concentric ring sources and the modified Bessel function respectively.

By fitting the experimental data to the straight line given by Eq. (7.91), the thermal conductivity is calculated and the thermal diffusivity is obtained from Eq. (7.87).

7.3.6

Discussion

These methods usually involve the heat source and the temperature sensor, embedded into materials. Depending on the size of the probe and of the specimen, materials with considerable inhomogeneities can be measured. The measurement process is characterized by the application of a small disturbance to a specimen held at a stable and uniform temperature. The disturbance is applied in the form of a heat pulse or a heat flux. The temperature–time response is recorded.

The thermal probe is particularly suitable for liquids, powders and moist materials. Although limitations are present, as far as *in situ* and field measurements are concerned the thermal probe is still a useful device. Experimental configurations can be designed such that the fulfillment of the requirements for applicability is attained by choice of appropriate specimen and probe sizes. Theoretically, an infinite line source and an infinite medium are necessary; therefore, the probe designed must have a reasonable length to diameter ratio. The thermal probe covers an approximate range of thermal conductivity of materials from 0.05 to 20 W m⁻¹ K⁻¹, whereas TPS covers a very broad range and is also useful for measurement on specimens available in various forms and sizes. The TPS method is capable of measuring thermal conductivity, thermal diffusivity and specific heat of materials simultaneously from cryogenic to high temperatures.

Acknowledgment

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8

Thermal Property of Lotus-Type Porous Copper and Application to Heat Sinks

Tetsuro Ogushi, Hiroshi Chiba, Masakazu Tane, and Hideo Nakajima

8.1

Introduction

As semiconductor chips generate heat due to Joule loss, heat sinks are usually used in semiconductor devices to reduce the temperature of the chips and obtain normal operation of the devices. Since the heat dissipation rates in powered devices and high-frequency electronic devices have been increasing in recent years, heat sinks with larger heat transfer performance have been required to cool these devices. Heat sinks utilizing microchannels with channel diameters of several tens of micrometers are expected to have a high cooling performance because a larger heat transfer capacity is obtained as the channel diameter becomes smaller.

The heat transfer performance of microchannels constructed in silicon wafers has been studied [1,2], and heat sinks utilizing microchannels with channel diameters of several tens of micrometers are expected to have a good cooling performance. To enhance the cooling performance of heat sinks with microchannels, three-dimensional stacked microchannel heat sinks have been investigated by Wei and Joshi [3]. Porous materials are considered to be preferable as three-dimensional microchannels. Bastawros and Evans [4] have investigated cellular metal as a heat transfer medium. Among various types of porous materials such as sintered porous metals, cellular metals and fibrous composites, lotus-type porous metals with straight pores are preferable for heat sinks due to a smaller pressure drop in cooling water flowing through straight pores.

Lotus-type porous copper has been investigated in microchannel heat sinks by Ogushi and co-workers [5,6]. An outer view of the lotus-type porous copper is shown in Figure 8.1a. It is made of copper with many straight pores that are formed by precipitation of supersaturated gas dissolved in the melted copper during solidification. Such lotus-type porous metals have been fabricated by Czochralski, casting and zone melting methods [7]. The primary features of lotus metals are: (a) straight pores, (b) pore size and porosity are controllable, and (c) possibility of producing porous metals with pores down to tens of micrometers in diameter.

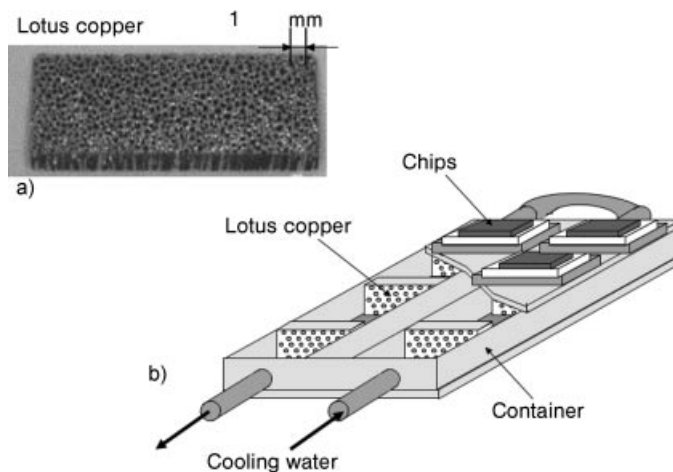


Figure 8.1 (a) Lotus-type porous copper and (b) lotus copper heat sink utilizing lotus-type porous copper.

To use lotus copper effectively in heat sinks, it is very important to know its effective thermal conductivity, considering the pore effect on the heat flow. There is a large literature devoted to the effective thermal conductivity of composite materials with cylindrical inclusions. Behrens [8] analytically investigated the effective thermal conductivities of composite materials under the assumption of orthorhombic symmetry and proposed a simple equation for predicting the effective thermal conductivity. Perrins *et al.* [9] proposed a method for predicting transport properties including the thermal conductivity of circular cylinders in square and hexagonal arrays. Han and Cosner [10] conducted a numerical investigation into the effective thermal conductivities of composites with uniform fibers in a unidirectional orientation and layered composites with fibers laid alternately along two mutually perpendicular directions. A numerical method has been developed by Sangani and Yao [11] to determine the effective thermal conductivity of a composite medium consisting of parallel circular cylinders in random arrays. They noted that the conductivity appeared to be a relatively weak function of the detailed arrangement of the cylinders. Mityushev [12] renewed the analysis of the resolution of the Laplace equation in composite materials with a collection of non-overlapping, identical, circular disks. Moctezuma-Berthier *et al.* [13] showed the predominant influence of the total porosity on the thermal properties of coarse porous media.

In the work reported in this chapter, we firstly investigated the effective thermal conductivities parallel and perpendicular to the pore axis of lotus copper both experimentally and analytically. As the thermal conductivity of the fluid in the pores is negligible in comparison with that of the lotus copper material in the application of the lotus copper to heat sinks, a very simple equation can be derived for the thermal conductivities of lotus copper.

Secondly, a straight fin model for predicting the heat transfer capacity of the lotus copper heat sink shown in Figure 8.1b was investigated. The heat conduction in the

porous metal and the heat transfer to the fluid in the pores are taken into consideration in the fin model. The model is compared with the numerical analysis in which the spacing between pores and the heat transfer coefficient in the pores are changed.

Finally, we examined experimentally and analytically the heat transfer capacities of three types of heat sink with conventional groove fins, with groove fins having a smaller fin gap (microchannels) and with lotus-type porous copper fins. Correlations for predicting the heat transfer capacity of these heat sinks are presented.

8.2

Effective Thermal Conductivity of Lotus-Type Porous Copper

8.2.1

Measurement

8.2.1.1 Definition of Effective Thermal Conductivity

The effective thermal conductivity of lotus copper k_{eff} is defined by

$$q = \frac{Q}{A} = -k_{\text{eff}} \cdot \nabla T \quad (8.1)$$

where q is a heat flux that is given from the heat flow Q divided by heat flowing through the cross-sectional area A in the lotus copper including pores, and T is the temperature in the lotus copper. The tensor k_{eff} is orthorhombic and is expressed as

$$k_{\text{eff}} = \begin{pmatrix} k_{\text{eff} //} & & \\ & k_{\text{eff} \perp} & \\ & & k_{\text{eff} \perp} \end{pmatrix} \quad (8.2)$$

The effective thermal conductivity of the lotus copper is anisotropic. The parallel and perpendicular effective thermal conductivities $k_{\text{eff} //}$, $k_{\text{eff} \perp}$ of the lotus copper are defined as the thermal conductivities for heat flow parallel and perpendicular to the pore axis, respectively, as shown in Figure 8.2.

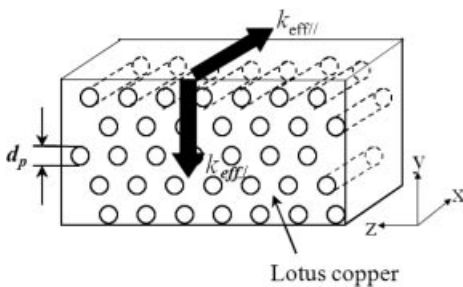


Figure 8.2 Definition of the effective thermal conductivity.

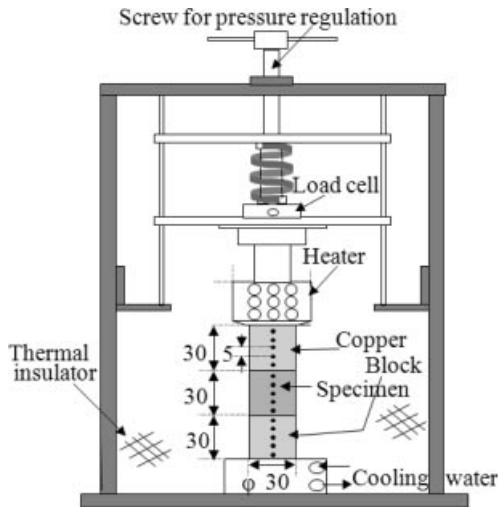


Figure 8.3 Experimental apparatus for measuring the effective thermal conductivity.

8.2.1.2 Experimental Method

Figure 8.3 presents the experimental apparatus for measuring the effective thermal conductivity. A cylindrical specimen with a diameter of 30 mm and a length of 30 mm was located between upper and lower copper rods of known thermal conductivity. The upper rod was heated by electrical heaters from the top surface, while the bottom surface of the lower rod was cooled by cooling water in order to transmit a certain amount of heat through the specimen. K-type thermocouples were located each at 5 mm spacing in the specimen and the upper and the lower rods to measure the temperature.

An example of the temperature distribution of the experimental set up is shown in Figure 8.4. As the heat flowed to one direction through the rods and specimen from

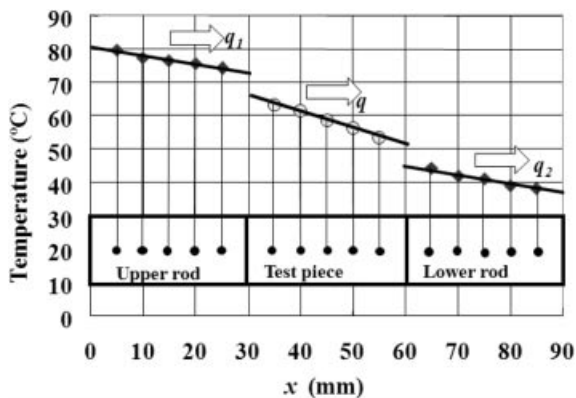


Figure 8.4 Temperature distribution in specimen and rods of experimental setup.

top to bottom, the heat flux q through the specimen was obtained by the following one dimensional equations:

$$q = \frac{q_1 + q_2}{2} \quad (8.3)$$

$$q_1 = -k_{\text{Cu}} \left(\frac{\partial T}{\partial x} \right)_1 \quad (8.4)$$

$$q_2 = -k_{\text{Cu}} \left(\frac{\partial T}{\partial x} \right)_2 \quad (8.5)$$

where q_1 is a heat flux from the upper rod to the specimen, q_2 is the heat flux from the specimen to the lower rod, T is the temperature, k_{Cu} is the thermal conductivity of the rods and x is the heat flow direction from upper to lower rod.

From Eqs. (8.1) to (8.5), the effective thermal conductivities $k_{\text{eff} //}$, $k_{\text{eff} \perp}$ are obtained by the following equation:

$$k_{\text{eff} //}, k_{\text{eff} \perp} = \frac{q_1 + q_2}{2 \left(\frac{\partial T}{\partial x} \right)_{\text{lotus}}} \quad (8.6)$$

where $(\partial T / \partial x)_{\text{lotus}}$ is the temperature gradient in the specimen with pores parallel or perpendicular to heat flow direction x . The experimental accuracy was evaluated as $\pm 10\%$.

8.2.1.3 Specimen Preparation

Lotus-type porous copper rods with long pores and various porosities were prepared by unidirectional solidification in a hydrogen and argon atmosphere; the detailed fabrication technique has been given by Hyun *et al.* [14]. The specimens were cut by spark erosion and machined into cylindrical shapes with the surface parallel or perpendicular to the pore axis.

The specifications of the lotus copper specimens are compiled in Table 8.1. Two types of lotus copper with pores parallel and perpendicular to the heat flow direction

Table 8.1 Specification of test pieces for measuring the effective thermal conductivity.

Heat flow direction	No.	Porosity	d_{pmax} (mm)	d_{pmin} (mm)	d_{pmean} (mm)	Mean distance between pore centers (mm)
Parallel	1	0.24	0.31	0.02	0.10	0.18
	2	0.28	0.36	0.04	0.13	0.21
	3	0.36	0.31	0.06	0.12	0.17
	4	0.43	0.17	0.02	0.08	0.11
Perpendicular	5	0.28	0.36	0.04	0.13	0.21
	6	0.31	0.29	0.05	0.13	0.20
	7	0.36	0.31	0.06	0.12	0.17

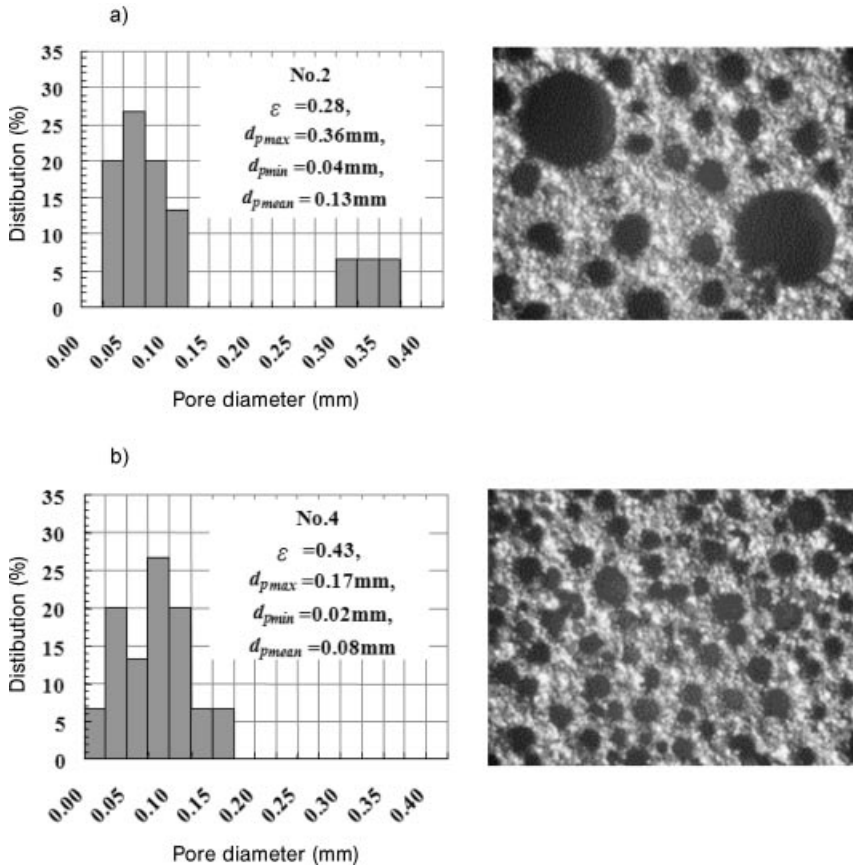


Figure 8.5 Microscopic view of specimens and distributions of pore diameters: (a) specimen no. 2, (b) specimen no. 4.

were measured, and the porosity of the specimens varied between 0.24 and 0.43. Figures 8.5a and b show the distribution of the pores and microscopic views of specimens 2 and 4. Specimen 2 has a bimodal distribution of the pore size. Since the diameters of the specimens were distributed around a certain range, the maximum diameter d_{pmax} , minimum diameter d_{pmin} , mean diameter d_{pmean} and distance between pore centers calculated from the assumption of the square array of pores are also noted in Table 8.1.

8.2.2

Thermal Conductivity Parallel to Pores

Since the heat flow cross-sectional area parallel to the pore axis in the lotus copper is proportional to $(1 - \varepsilon)$, the effective thermal conductivity $k_{eff//}$ is expressed as the following equation:

$$\frac{k_{\text{eff} //}}{k_s} = 1 - \varepsilon \quad (8.7)$$

where k_s is the thermal conductivity of the nonporous copper and ε is the porosity expressed by the volume ratio of pores against the total volume of the lotus copper.

Figure 8.6 shows a comparison between the experimental data and the results evaluated by the analytical Eq. (8.7) for the thermal conductivity parallel to the pores. Experimental data for $k_{\text{eff} //}$ showed good agreement with the analytical results derived from the assumption that heat flow through the cross-sectional area parallel to the pore axis is proportional to $(1 - \varepsilon)$. The value of $335 \text{ W m}^{-1} \text{ K}^{-1}$ as the thermal conductivity k_s of the lotus copper material was used for comparison.

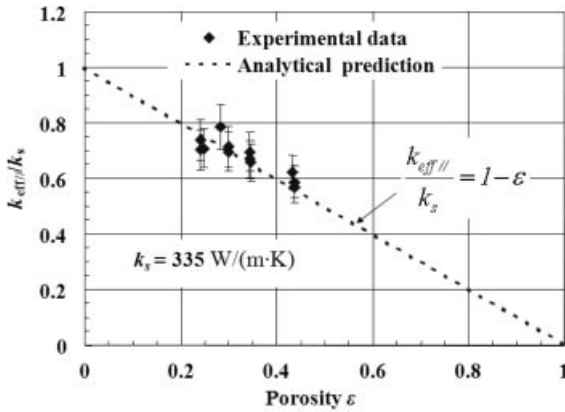


Figure 8.6 Comparison of experimental data of the effective thermal conductivity of lotus copper parallel to pores with analysis data of Eq. (8.7).

8.2.3

Thermal Conductivity Perpendicular to Pores

Behrens [8] derived the effective thermal conductivity of composite materials with orthorhombic symmetry. By applying his equation to the thermal conductivity of the lotus copper, the effective thermal conductivity perpendicular to the pores can be expressed by the following equation:

$$\frac{k_{\text{eff} \perp}}{k_s} = \frac{(\beta + 1) + \varepsilon(\beta - 1)}{(\beta + 1) - \varepsilon(\beta - 1)} \quad (8.8)$$

where $\beta (= k_p / k_s)$ is the conductivity ratio, that is, the pore conductivity k_p divided by the material conductivity k_s of the lotus copper.

Because the thermal conductivity of the hydrogen gas or air in the pores of the lotus copper is negligible compared with that of the lotus material, the effective

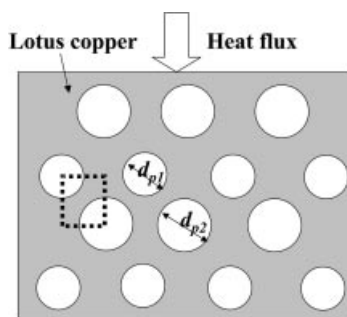


Figure 8.7 Numerical simulation model of lotus copper.

thermal conductivity of the lotus copper can be expressed as the following equation by setting $\beta = 0$ in Eq. (8.8):

$$\frac{k_{\text{eff} \perp}}{k_s} = \frac{1 - \varepsilon}{1 + \varepsilon} \quad (8.9)$$

Han and Cosner [10] have performed a numerical study on the effective thermal conductivities of fibrous composites by using a unit cell approach under a uniform fiber diameter condition. Since the diameter of the lotus copper is distributed around a certain range, a numerical simulation for the thermal conductivity perpendicular to the pores under a nonuniform pore diameter condition was conducted to verify the applicability of Eq. (8.9) to the lotus copper.

Figure 8.7 shows that the lotus copper contained many pores of different diameters. The pores were assumed to be circular in cross-section but of different diameters and aligned in a uniform staggered array in the numerical simulation. A unit cell model including double pores with different pore diameters of d_{p1} and d_{p2} in a square with side length w was used in the simulation, as shown in Figure 8.8.

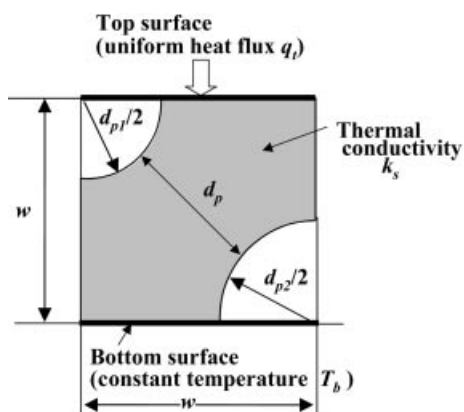


Figure 8.8 Unit cell model for numerical simulation of the effective thermal conductivity perpendicular to round pores.

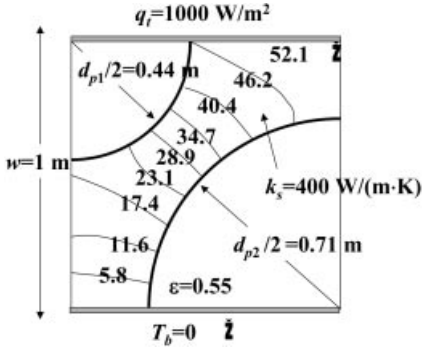


Figure 8.9 Temperature distribution in the unit cell model for round pores.

The mean temperature difference ΔT_m between top and bottom surfaces was calculated using the finite difference method under the following boundary condition: input uniform heat flux q at the top surface and a constant temperature T_b at the bottom surface. In the calculation, d_{p2} was changed under three sets of constant $(d_{p1}/2)/w = 0.26, 0.44, 0.65$.

An example of the temperature distribution in the unit cell model is shown in Figure 8.9. The temperatures at the top surface were higher than those of the bottom surface, and the mean temperature difference ΔT_m between the top and the bottom surface was obtained from the temperature distribution in the model.

The effective thermal conductivity perpendicular to the round pores is calculated from the following equation:

$$k_{\text{eff} \perp} = \frac{q(w - d_{p1}/2)}{\Delta T_m} \quad (\text{round pores}) \quad (8.10)$$

The porosity ε is calculated from the following equation:

$$\varepsilon = \frac{\frac{\pi}{4} \left\{ \left(\frac{d_{p2}}{2} \right)^2 + \left(\frac{d_{p1}}{2} \right)^2 \right\}}{w^2} \quad (\text{round pores}) \quad (8.11)$$

Figure 8.10 shows a comparison of the numerically simulated results with the analytical results from Eq. (8.9), shown by a dotted line for the effective thermal conductivity perpendicular to the pores. The analytical Eq. (8.9) showed good agreement with the numerical simulation, which means that Eq. (8.9), derived from the assumption of orthorhombic symmetry, can be used to predict the effective thermal conductivity perpendicular to pores under a uniform, staggered array with a non-uniform pore diameter condition.

Figure 8.11 shows a comparison between the experimental data and Eq. (8.9), where the effective thermal conductivity $k_{\text{eff} \perp}$ perpendicular to the pores was lower than that parallel to the pores ($k_{\text{eff} \parallel}$), and was 40% of the lotus copper material k_s with a porosity of 0.4. The analytical values evaluated by Eq. (8.9) showed good

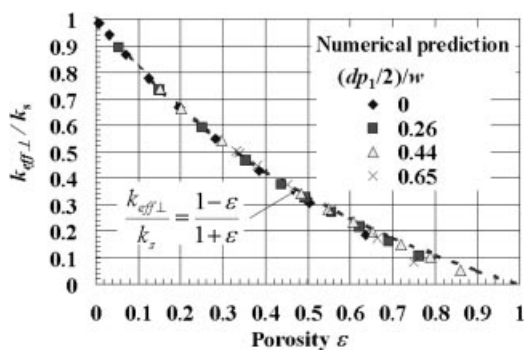


Figure 8.10 Comparison of numerical results of the effective thermal conductivity of lotus copper perpendicular to round pores with analysis data of Eq. (8.9).

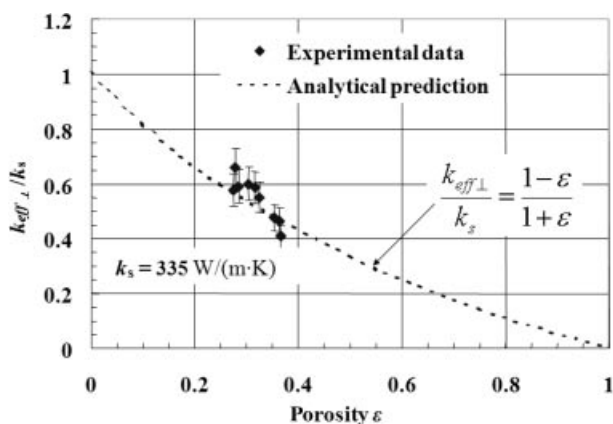


Figure 8.11 Comparison of experimental data of the effective thermal conductivity of lotus copper perpendicular to pores with analysis data of Eq. (8.9).

agreement with the experimental data, indicating that Eq. (8.9) can be used to predict the effective thermal conductivity perpendicular to pores of lotus copper within an experimental accuracy of $\pm 10\%$.

The results from Figures 8.6 and 8.11 show that the lotus copper displayed anisotropy of the effective thermal conductivity. The effective thermal conductivity $k_{eff\perp}$ perpendicular to pores was lower than that parallel to the pores $k_{eff\parallel}$.

8.2.4

Effect of Pore Shape on Thermal Conductivity

Since the diameter of the pores of the lotus metal is distributed around a certain range and the cross-sectional shape of pores is not necessarily circular, a numerical simulation for effective thermal conductivity perpendicular to the pores with a

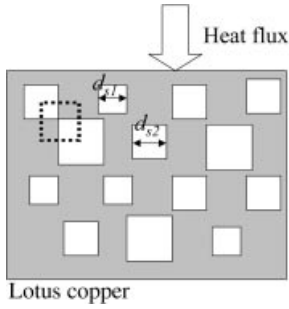


Figure 8.12 Numerical simulation model of lotus copper containing many pores of square shape.

nonuniform pore diameter and different pore shape was conducted to verify the applicability of Eq. (8.9) to lotus copper.

Figure 8.12 shows the numerical simulation model of lotus copper. The pores were assumed to be square in cross-sectional shape with various different sizes, and aligned in a uniform staggered array in the numerical simulation. A unit cell model that included double pores with different side lengths of d_{s1} and d_{s2} in a square with side length of w was used in the simulation, as shown in Figure 8.13. The difference of mean temperature ΔT_m between the top and bottom surfaces of the unit cell was calculated by using the finite difference method under the following boundary conditions: input uniform longitudinal heat flux q_t at the top surface and uniform temperature T_b at the bottom surface. In the calculation, d_{s2} was changed for four sets of constant $(d_{s1}/2)/w$ under condition $0.1 < d_s/w < 1$, where $d_s = w - d_{s1}/2 - d_{s2}/2$.

An example of the temperature distribution in the unit cell model is shown in Figure 8.14. The temperatures at the top surface were higher than those at the bottom surface, and the difference in temperature between the top and bottom surfaces of the unit cell ΔT_m was obtained from the temperature distribution in the model.

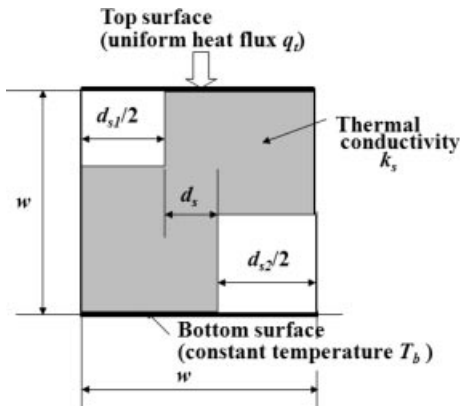


Figure 8.13 Unit cell model for numerical simulation of the effective thermal conductivity perpendicular to square pores.

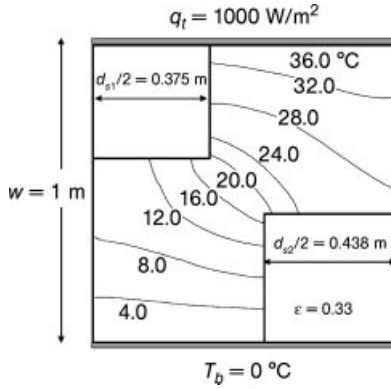


Figure 8.14 Temperature distribution in the unit cell model for square pores.

The effective thermal conductivity perpendicular to the square pores is calculated using

$$k_{\text{eff} \perp} = \frac{q(w - d_{s1}/2)}{\Delta T_m} \quad (\text{square pores}) \quad (8.12)$$

The porosity ε is calculated from the following equation for square pores:

$$\varepsilon = \frac{\left(\frac{d_{s1}}{2}\right)^2 + \left(\frac{d_{s2}}{2}\right)^2}{w^2} \quad (\text{square pores}) \quad (8.13)$$

Figure 8.15 compares the numerical results with those evaluated by both the analytical Eq. (8.9) (solid line) and a value 10% less than Eq. (8.9) (dotted line) for

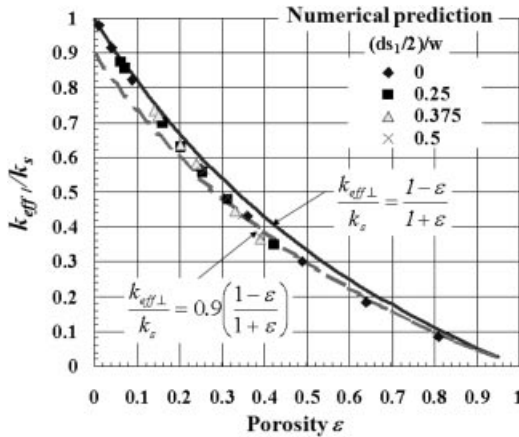


Figure 8.15 Comparison between numerical and evaluated results by the analytical equation (8.9) for square pores.

the effective thermal conductivity perpendicular to the square pores as a function of porosity. As for square pores, Eq. (8.9) gave higher values of the effective thermal conductivity than the numerical results, showing less than 10% discrepancy. Conclusively, the effective thermal conductivity perpendicular to the pores of the lotus metal can be predicted within 10% discrepancy by Eq. (8.9) as a function of porosity, even if the pore shape is not circular and the pore size is not uniform.

8.2.5

Effect of Pore Orientation on Thermal Conductivity

8.2.5.1 Introduction

The pores of lotus metals are anisotropic. Therefore, in order to clarify their anisotropic thermal conductivity, it is necessary to examine the thermal conductivity not only in the directions parallel and perpendicular to the pore direction but also in the other directions. Furthermore, misorientation of pores occurs in lotus metals. However, this effect on the effective thermal conductivity has not been studied. The theory of Hatta and Taya [15,16], based on Eshelby's inclusion theory [17] and mean-field theory [18], can provide the effective conductivity of composites with misoriented inclusions. However, the mean-field theory is not adequate when applied to composites with inclusions of high volume fraction. This is a shortcoming of the Hatta–Taya theory. In order to overcome this problem, Tane *et al.* [19] have proposed the extended effective mean-field (EMF) theory by combining the Hatta–Taya theory and the effective-medium approximation [20]. The extended EMF theory can validly take into account the effect of misoriented inclusions even where the volume fraction of inclusions is high.

Tane *et al.* applied the extended EMF theory to lotus metals, and examined the effect of the direction of applied temperature gradient (electric field [19]) and pore orientation on the effective thermal (electrical [19]) conductivity.

8.2.5.2 EMF Theory

The EMF theory for the effective elastic constants of composite materials [21–23] was proposed by Tane *et al.*, and the concept was also applied to effective conductivity including electrical, thermal conductivities, etc. [17,22]. The effective thermal conductivity of composite materials with misoriented inclusions, $\bar{k}_{(n+1)}$, is given by [19]

$$\bar{k}_{(n+1)} = \bar{k}_{(n)} + \frac{\Delta f}{1-n\Delta f} \left[\langle k_I A_{(n)}^{MT} \rangle - \bar{k}_{(n)} \langle A_{(n)}^{MT} \rangle \right] \quad (8.14)$$

where $\bar{k}_{(n+1)}$ and $\bar{k}_{(n)}$ are the effective thermal conductivities of composite materials with inclusions of $(n+1)\Delta f$ and $n\Delta f$, respectively; k_I is the thermal conductivity of inclusions (k is given in the form of a 3×3 matrix, and the components are 0 when $i \neq j$). The term Δf is given by $\Delta f = 1/N \ll 1$, where the value of N is integer (in the present study, the value of Δf is 0.01). Successive calculations using Eq. (8.14)

provide $\bar{\mathbf{k}}_{(n+1)}$ of composite materials with inclusions of various volume fractions, where $\bar{\mathbf{k}}_{(0)} = \mathbf{k}_M$ and $\bar{\mathbf{k}}_{(N)} = \mathbf{k}_I$. The terms $\langle \mathbf{k}_I \mathbf{A}_{(n)}^{\text{MT}} \rangle$ and $\langle \mathbf{A}_{(n)}^{\text{MT}} \rangle$ are expressed as

$$\langle \mathbf{k}_I \mathbf{A}_{(n)}^{\text{MT}} \rangle = \left\langle \mathbf{k}_I \mathbf{A}_{(n)}^{\text{dil}} \left[\left(1 - \frac{\Delta f}{1 - n\Delta f} \right) \mathbf{I} + \frac{\Delta f}{1 - n\Delta f} \mathbf{k}_I \mathbf{A}_{(n)}^{\text{dil}} \right]^{-1} \right\rangle \quad (8.15)$$

$$\langle \mathbf{A}_{(n)}^{\text{MT}} \rangle = \left\langle \mathbf{A}_{(n)}^{\text{dil}} \left[\left(1 - \frac{\Delta f}{1 - n\Delta f} \right) \mathbf{I} + \frac{\Delta f}{1 - n\Delta f} \mathbf{k}_I \mathbf{A}_{(n)}^{\text{dil}} \right]^{-1} \right\rangle \quad (8.16)$$

where $\mathbf{A}_{(n)}^{\text{MT}}$ and $\mathbf{A}_{(n)}^{\text{dil}}$ of 3×3 matrix are, respectively, given by

$$\mathbf{A}_{(n)}^{\text{MT}} = \mathbf{A}_{(n)}^{\text{dil}} \left[\left(1 - \frac{\Delta f}{1 - n\Delta f} \right) \mathbf{I} + \frac{\Delta f}{1 - n\Delta f} \mathbf{A}_{(n)}^{\text{dil}} \right]^{-1}$$

and

$$\mathbf{A}_{(n)}^{\text{dil}} = \left[\mathbf{S}_{(n)} \bar{\mathbf{k}}_{(n)} (\mathbf{k}_I - \bar{\mathbf{k}}_{(n)}^{-1}) + \mathbf{I} \right]^{-1}$$

where $\mathbf{I}$ is the unit 3×3 matrix. The matrix $\mathbf{S}_{(i)}$ is the Eshelby tensor of 3×3 matrix, and it is a function of $\bar{\mathbf{k}}_{(n)}$. The Eshelby tensor $\mathbf{S}_{ij}$ for an ellipsoidal inclusion embedded in a medium with anisotropic thermal conductivity is given by [24]

$$\mathbf{S}_{ij} = \frac{a_1 a_2 a_3}{4\pi} \int_{S^2} \sigma_{mn} \bar{\xi}_i \bar{\xi}_m \zeta^{-3} (\sigma_{rs} \bar{\xi}_r \bar{\xi}_s)^{-1} dS(\bar{\xi}) \quad (8.17)$$

where the integration is performed over the unit sphere S^2 ; $\zeta^2 = a_1^2 \bar{\xi}_1^2 + a_2^2 \bar{\xi}_2^2 + a_3^2 \bar{\xi}_3^2$; a_1 , a_2 and a_3 are the radii of the ellipsoidal inclusion. When the shape of an inclusion is given by $a_3/a_1 (= a_2) \rightarrow \infty$, i.e. the shape is cylindrical, the Eshelby tensor is given by

$$\mathbf{S}_{ij} = \frac{1}{2\pi} \int_{S^L} \sigma_{mn} \bar{\xi}_i \bar{\xi}_m (\sigma_{rs} \bar{\xi}_r \bar{\xi}_s)^{-1} dL(\bar{\xi}) \quad (8.18)$$

where the integration is performed over the unit circle S^L normal to the x_3 direction.

8.2.5.3 Application of Extended EMF Theory to Lotus Metals

Tane *et al.* [19] applied the EMF theory to lotus metals, calculated the effective thermal conductivities in various directions and examined the effect of pore orientation on the effective thermal conductivity. In calculations with the EMF theory, lotus metals were modeled as follows:

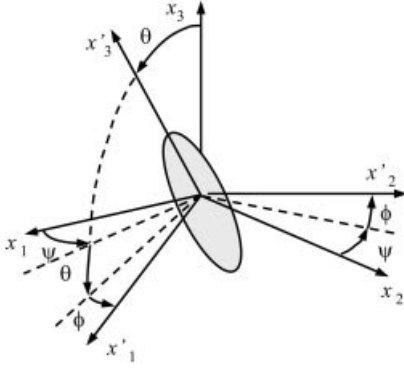


Figure 8.16 Schematic indicating a coordinate system of an ellipsoidal inclusion. The inclusion coordinate system is defined by the three Euler angles ψ , θ and ϕ , where x and x' are the coordinate system of a matrix and inclusion, respectively. The longitudinal axis of the ellipsoid is parallel to the x'_3 axis.

The thermal conductivity of a matrix is isotropic.

1. Since the thermal conductivity of pores is negligible compared with that of a metal matrix, the value is put equal to zero.
2. The pores are cylindrical, and the shape is expressed as $(x'^2_1 + x'^2_2)/a_1^2 + x'^2_3/a_3^2 \leq 1$ and $a_3/a_1 \rightarrow \infty$, where x' is the coordinate system of an inclusion.
3. The orientation of a pore is given by the Euler angles (θ , ψ and ϕ) defined in Figure 8.16. In the present study, the value of θ is fixed, and the values of ψ and ϕ are random. Since the orientation of pores is localized at a given θ , the following formula provides the orientation average of X_{ij} :

$$\langle X_{ij} \rangle = \frac{1}{4\pi^2} \int_0^{2\pi} d\psi \int_0^{2\pi} d\phi X_{ij}(\psi, \theta, \phi) \quad (8.19)$$

The procedure for calculating $\langle \mathbf{k}_l \mathbf{A}_{(n)}^{\text{MT}} \rangle$ and $\langle \mathbf{A}_{(n)}^{\text{MT}} \rangle$ in Eqs. (8.15) and (8.16) is outlined below:

1. Calculate the Eshelby tensors S'_{pq} of all inclusions in their coordinate systems identified by the Euler angles (θ , ψ and ϕ), using Eq. (8.18). Convert their coordinate systems to a matrix coordinate system using $S_{ij}(\psi, \theta, \phi) = a_{ip} a_{jq} S'_{pq}$ where a_{ip} is the component of a rotation conversion matrix consisting of ψ , θ and ϕ .
2. Calculate $\mathbf{A}_{(n)}^{\text{dil}}$ by using the converted S_{ij} and the equation

$$\mathbf{A}_{(n)}^{\text{dil}} = \left[\mathbf{S}_{(n)} \bar{\mathbf{k}}_{(n)}^{-1} (\mathbf{k}_l - \bar{\mathbf{k}}_{(n)}) + \mathbf{I} \right]^{-1}$$

3. Calculate $k_l A_{(n)}^{MT}$ and $A_{(n)}^{MT}$ by using the calculated $A_{(n)}^{dil}$ and the equation

$$A_{(n)}^{MT} = A_{(n)}^{dil} \left[\left(1 - \frac{\Delta f}{1 - n\Delta f} \right) I + \frac{\Delta f}{1 - n\Delta f} A_{(n)}^{dil} \right]^{-1}$$

4. Calculate $\langle k_l A_{(n)}^{MT} \rangle$ and $\langle A_{(n)}^{MT} \rangle$ by using the calculated $k_l A_{(n)}^{MT}$, $A_{(n)}^{MT}$ and Eq. (8.15) or Eq. (8.16).

Effective Thermal Conductivity in Various Directions The effective thermal conductivity of a typical lotus metal with perfectly aligned pores ($\theta = 0^\circ$) was calculated, where coordinate conversion of the calculated effective thermal conductivities provides the conductivities in various directions. Figure 8.17 shows the normalized effective thermal conductivity, $\bar{k}/k_M$, of the lotus metal with $\varepsilon = 0.40$ in the direction of ω from the x_3 axis, where the definition of ω is the same as that of θ . Since the thermal conductivity of the matrix is isotropic, it is expressed by k_M , a scalar quantity. The normalized conductivity $\bar{k}/k_M$ decreases with increasing ω . This is because the distance of the path that the thermal flux flows increases with increasing ω . The thermal conductivity in the directions near $\theta = 0$ and 90° is insensitive to the angle ω . These trends are common to lotus metals with various porosities.

Effect of Misorientation of Pores on the Effective Thermal Conductivity The effective thermal conductivity of lotus metals of $\theta = 0, 10$ and 20° was calculated. Figure 8.18 shows the porosity dependence of $k_{eff\perp}/k_M$ and $k_{eff\parallel}/k_M$, where $k_{eff\perp}$ and $k_{eff\parallel}$ are conductivities in the directions perpendicular and parallel to the pores. The effective thermal conductivity in the direction parallel to the pore direction is more

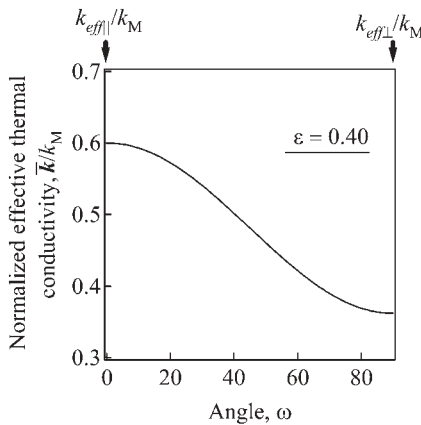


Figure 8.17 Normalized effective thermal conductivity, $\bar{k}/k_M$, of a lotus metal of $\theta = 0^\circ$ and $\varepsilon = 0.40$ in the direction of ω from the x_3 axis.

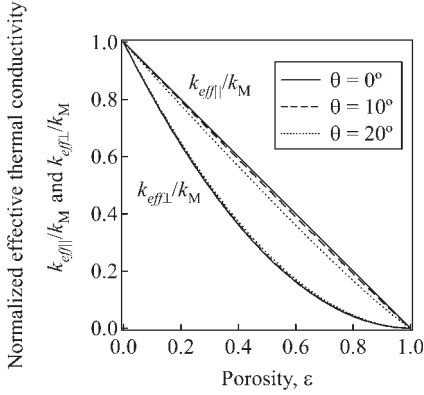


Figure 8.18 Normalized thermal conductivities of lotus metals in the direction parallel and perpendicular to the x_3 axis: $k_{\text{eff}\perp}/k_M$ and $k_{\text{eff}\parallel}/k_M$, where $\theta = 0, 10$ and 20° .

sensitive to the misorientation of pores than that in the parallel direction. When $\theta = 20^\circ$, the porous morphology slightly deviates from the typical lotus-type structure of $\theta = 0^\circ$; however, the effective thermal conductivity for $\theta = 20^\circ$ is almost the same as that for $\theta = 0^\circ$. This indicates that the slight deviation of pore morphology hardly affects the effective thermal conductivity of lotus metals.

8.3

Application of Lotus-Type Porous Copper to Heat Sinks

8.3.1

Analysis of Fin Efficiency

8.3.1.1 Straight Fin Model

In order to predict the heat transfer capacity of lotus copper, the heat conduction in the porous metal and the heat transfer to the fluid in the pores must be taken into consideration. In the lotus-type porous copper heat sink, heat is input from the top surface and flows downward by heat conduction with the heat transfer to the fluid in the pores as shown in Figure 8.19a. The lotus copper fin is modeled as a straight fin as shown in Figure 8.19b. The heat transfer rate Q under the temperature difference ΔT between the top surface of the fin and the fluid in the pores is calculated from

$$Q = hS_f\eta\Delta T \quad (8.20)$$

where η is the fin efficiency, S_f is the total surface area of pores and h is the heat coefficient in the pores.

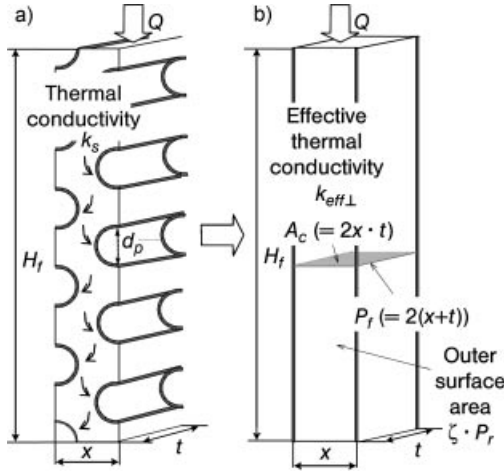


Figure 8.19 Analytical fin model: (a) lotus copper fin model, (b) straight fin model.

In the straight fin, the fin efficiency is expressed as follows:

$$\eta = \frac{\tanh(mH_f)}{mH_f} \quad (8.21)$$

$$m = \sqrt{\frac{h\zeta P_f}{k_{eff\perp} A_c}} \quad (8.22)$$

where H_f is the fin height, $k_{eff\perp}$ is the effective thermal conductivity perpendicular to the pore axis, P_f is the peripheral length of the fin, A_c is the cross-sectional area of the fin and ζ is the ratio between the total surface area of the lotus copper S_f and the total surface area of the straight fin $P_f H_f$, which can be expressed as

$$\zeta = \frac{S_f}{P_f H_f} \quad (8.23)$$

8.3.1.2 Numerical Analysis

In order to verify the efficiency of the straight fin model, numerical analysis for predicting the fin effectiveness was conducted. The numerical model of the lotus copper is shown in Figure 8.20.

The mean temperature ΔT between the top surface of the fin model and surrounding temperature T_s in the pores was calculated using finite difference method under the following boundary condition: uniform heat input Q at the top surface, uniform heat transfer coefficient h in the pores and constant surrounding temperature T_s .

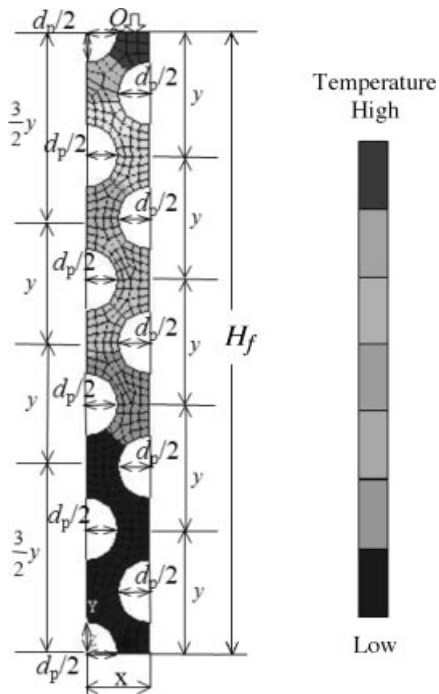


Figure 8.20 Numerical model to predict fin efficiency.

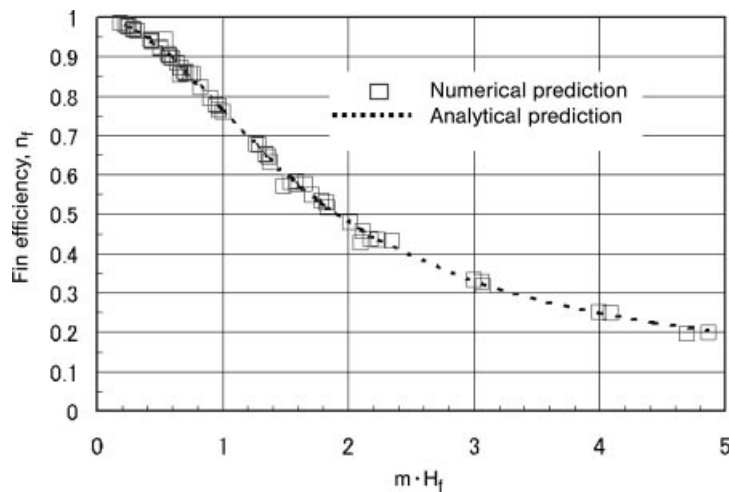


Figure 8.21 Comparison of fin efficiency between numerical and analytical prediction from Eq. (8.3).

In the calculation, a spacing of pores x , y was changed under uniform pore diameter d_p of $200\text{ }\mu\text{m}$ and material thermal conductivity k_s of $400\text{ W m}^{-1}\text{ K}^{-1}$.

The comparison of the fin efficiency η between the numerical results and results from Eq. (8.21) is shown in Figure 8.21. Equation (8.21) showed good agreement with the numerical simulation. Thus, the fin efficiency of the lotus fin η was verified to be predictable by Eq. (8.21) derived from the straight fin model.

8.3.2

Experiments of Heat Transfer Characteristics

8.3.2.1 Experimental Method

The experimental apparatus for measuring the heat transfer capacity of heat sinks is shown in Figure 8.22. Cooling water was circulated through a filter and the test duct in which the heat sink is located. The circulator has a pump and equipment for water-cooling. The heat sink consisted of fins that are brazed on one side of a copper base plate. The heating block with a heater was soldered on the other side of the base plate. The inlet temperature of cooling water T_i , the temperature of the copper base plate T_b and the outlet temperature of cooling water T_o were measured by K-type thermocouples. The heat transfer capacity was evaluated by a heat transfer h_i based on the base plate area A_b as follows:

$$h_i = \frac{Q}{A_b(T_b - T_i)} \quad (8.24)$$

where Q is the heat transfer rate that is evaluated from the heat input by reducing the heat loss through the thermal insulator around the heater from the heat input. The

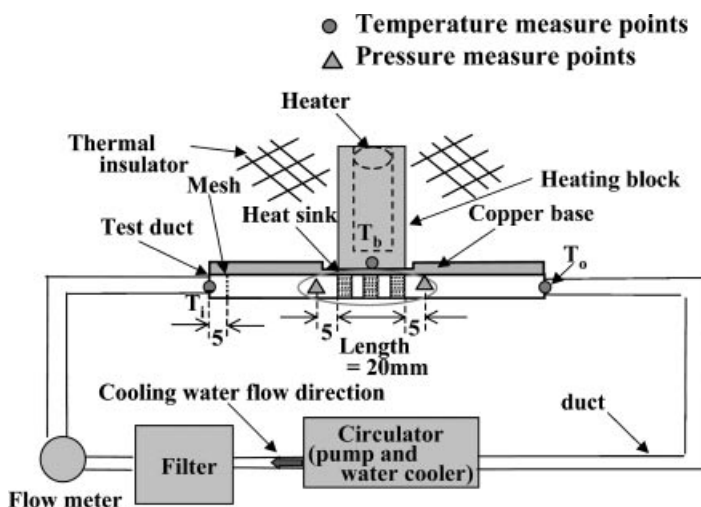


Figure 8.22 Schematic of experimental apparatus for measuring heat transfer capacity.

pressure drop between the inlet and the outlet of the fins of every heat sink was measured within an experimental accuracy of $\pm 5\%$ using a pressure sensor (Krone Corp, model DP-15).

8.3.2.2 Investigated Heat Sinks

The heat transfer capacities of the three types of heat sinks with conventional groove fins, groove fins with smaller fin gap (microchannel) and lotus-type porous copper were investigated. The configuration and the specifications of the conventional groove fins and microchannels are shown in Figure 8.23 and Table 8.2. The conventional groove fins have a fin gap of 3 mm and fin thickness of 1 mm. The microchannels have fin gap of 0.5 mm and fin thickness of 0.5 mm. The heat transfer capacity of the conventional groove fins is only for calculation.

The configuration of the lotus-type porous copper heat sink is shown in Figure 8.24. The heat sink has three pieces of lotus copper fins of length of 3 mm along the flow direction. The lotus-type porous copper fins have pores with mean diameter of 0.3 mm and porosity of 0.39.

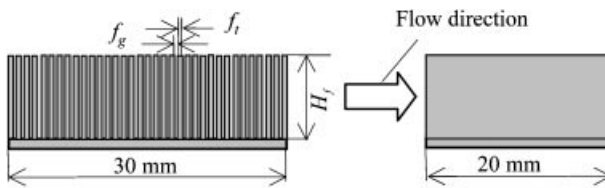


Figure 8.23 Conventional groove fins and microchannels.

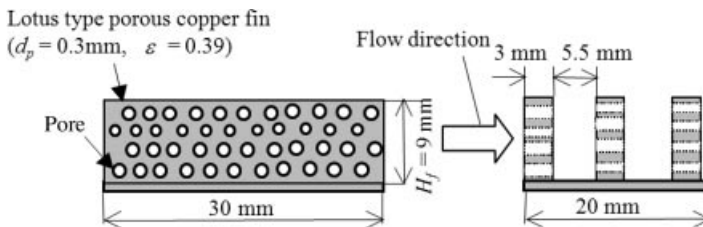


Figure 8.24 Lotus-type porous copper heat sink.

Table 8.2 Specification of conventional groove fins and microchannels.

	Fin gap, f_g (mm)	Fin thickness, f_t (mm)	Fin height, H_f (mm)	Investigation
Conventional groove fins	3	1	9	Calc.
Microchannels	0.5	0.5	9	Calc. and measured

8.3.3

Predictions of Heat Transfer Characteristics**8.3.3.1 Conventional Groove Fins and Microchannels**

Correlations for heat transfer coefficient h and a pressure drop ΔP of the conventional groove fins and microchannels are expressed by the following equations in the laminar flow regime ($Re_g < 3000$) [25,26]:

$$Nu_g = \frac{Nu_1 - Nu_2}{10 - 0.71} (Pr - 0.71) + Nu_2 \quad (8.25)$$

$$Nu_1 = 2.80136 - 2.10514X^* + 0.411783X^{*2} + 4.11 \quad (8.26)$$

$$Nu_2 = 4.18880 - 3.14709X^* + 0.611075X^{*2} + 4.11 \quad (8.27)$$

$$X^* = \ln\left(\frac{L}{f_g} Re_g Pr\right) \quad (8.28)$$

where Re_g is the Reynolds number defined by the fin gap ($= uf_g/\nu$), Nu_g is the Nusselt number defined by the fin gap ($= hf_g/k_f$), L is the length of groove fin along flow direction, u is the velocity of a fluid through the fin gaps, ν is the dynamic viscosity of the fluid and k_f is the thermal conductivity of the fluid.

$$\Delta P = f \left(\frac{4L}{D_e} \right) \left(\frac{1}{2} \rho u^2 \right) \quad (8.29)$$

$$f = \frac{3.44}{X^{0.5} Re_d} + \frac{24 + \left(\frac{0.674}{4X} \right) - \left(\frac{3.44}{X^{0.5}} \right)}{(1 + 0.000029X^{-2}) Re_d} \quad (8.30)$$

$$X = L / (Re_d D_e) \quad (8.31)$$

where D_e is the hydraulic diameter of the fin gap ($= 4f_g H_f / 2(f_g + H_f)$) and Re_d is the Reynolds number defined by the hydraulic diameter D_e ($= u D_e / \nu$).

8.3.3.2 Lotus-Type Porous Copper Fins

As the flow characteristics through the pores in the lotus copper fins is considered to be similar to a circular pipe, the heat transfer coefficient and pressure drop of the lotus copper fins are expressed by the following correlations for a circular pipe in the laminar flow regime ($Re_p < 3000$) [27]:

$$Nu_p = 5.364(1 + \{(220/\pi)X^+\}^{-10/9})^{3/10} \left\{ 1 + \left(\frac{\pi/(115.2X^+)}{[1 + (Pr/0.0207)^{2/3}]^{1/2} [1 + \{(220/\pi)X^+\}^{-10/9}]^{3/5}} \right)^{5/3} \right\}^{3/10} - 1 \quad (8.32)$$

$$X^+ = (L/d_p)/(Re_p Pr) \quad (8.33)$$

$$\Delta P = \left(\frac{64}{Re_p}\right) \left(\frac{L}{d_p}\right) \left(\frac{1}{2} \rho u^2\right) \quad (8.34)$$

where Re_p is the Reynolds number ($= u d_p / \nu$) and Nu_p is the Nusselt number ($= h d_p / k_i$).

8.3.4

Comparison of Experiments with Predictions

The heat transfer coefficients h_i based on base plate surface area A_b defined by Eqs. (8.24) for experiment and (8.35) for prediction are plotted in Figure 8.25 for all of the heat sinks as a function of the inlet velocity to the heat sinks u_o :

$$h_i = \frac{1}{R_{bi} A_b} \quad (8.35)$$

where R_{bi} is the thermal resistance between base plate and inlet of cooling water. The thermal resistance R_{bi} is derived from the following equations:

$$R_{bi} = \frac{R_w}{1 - \exp\left(-\frac{R_w}{R_f}\right)} \quad (8.36)$$

$$R_f = \frac{1}{h S_f \eta} \quad (8.37)$$

$$R_w = \frac{1}{C_p \rho V} \quad (8.38)$$

where R_f is the thermal resistance between the base plate and cooling water in the pores, R_w is the thermal resistance caused by the temperature rise of the cooling water from the inlet, V is the flow rate, C_p is the specific heat and ρ is the density of cooling water.

The prediction for the lotus-type porous copper heat sink showed good agreement with the experimental data within an accuracy of $\pm 15\%$. The experimental data of the lotus-type porous copper heat sink showed a very large heat transfer coefficient of $80\,000 \text{ W m}^{-2} \text{ K}^{-1}$ under a velocity u_o of 0.2 m s^{-1} , that is, 1.7 times higher than that of the microchannels and 6.5 times higher than that of the conventional groove fins.

The pressure drops in all of the heat sinks are compared in Figure 8.26 as a function of u_o . The predicted pressure drop of the lotus-type porous copper heat sink showed good agreement with the experimental data within an accuracy of $\pm 5\%$. On

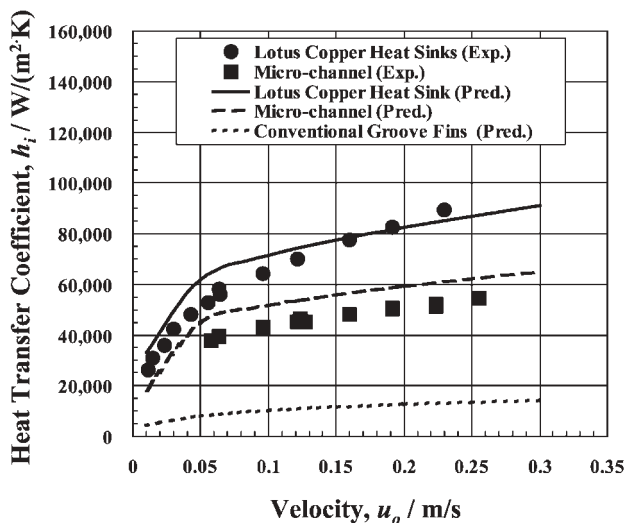


Figure 8.25 Comparison of heat transfer h_i between experimental and predicted data.

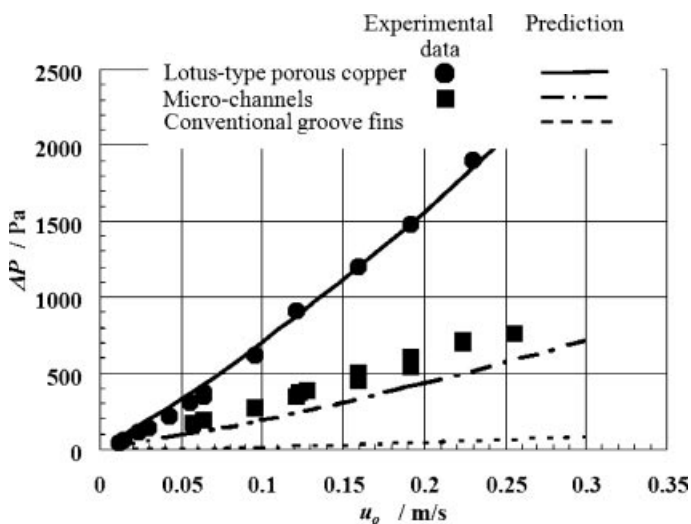


Figure 8.26 Comparison of pressure drop ΔP between experimental and predicted data.

comparing the pressure drop among all of the heat sinks under the velocity u_o of 0.2 m s^{-1} , the value of the lotus-type porous copper heat sink is 2.5 times higher than that of the microchannels and around 40 times higher than that of the conventional groove fins.

The heat transfer coefficient h_i as a function of ΔP is shown in Figure 8.27. Comparing the heat transfer coefficients among all of the heat sinks under the same pressure drop, the experimental value of the lotus-type copper heat sink is

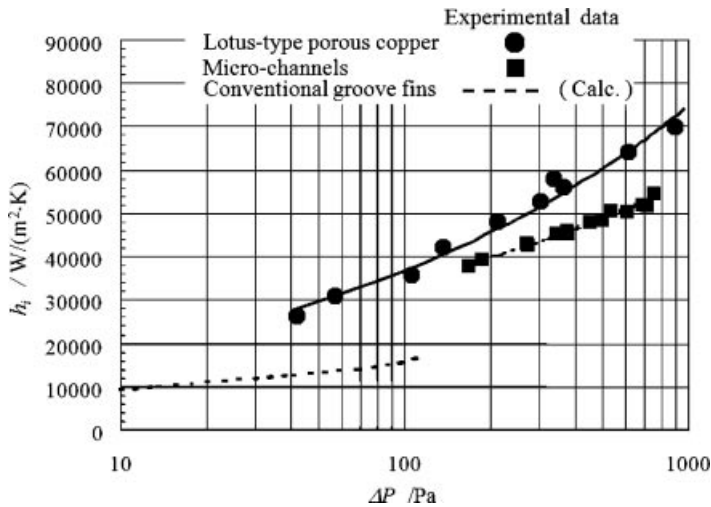


Figure 8.27 Comparison of heat transfer h_i as a function of pressure drop.

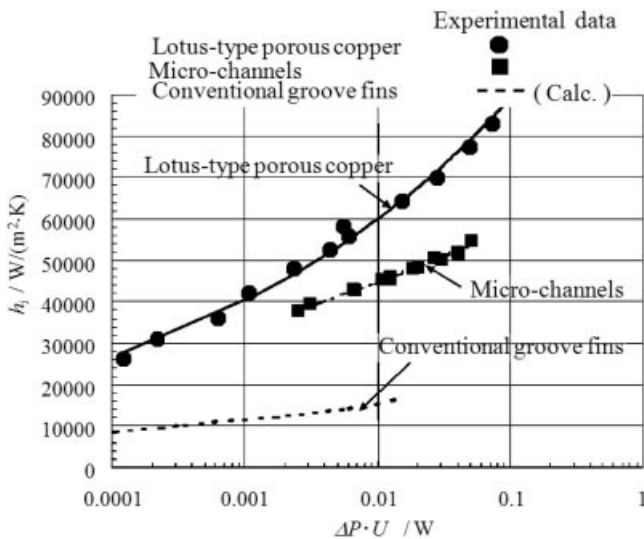


Figure 8.28 Comparison of heat transfer h_i as a function of pumping power.

around 1.2 times higher than that of the microchannels and 2 times higher than that of the conventional groove fins.

The heat transfer coefficient h_i as a function of pumping power that is defined by a product of a flow rate U and ΔP is shown in Figure 8.28. Comparing the heat transfer coefficients among all of the heat sinks under the pumping power of 0.01 W, the experimental value of the lotus-type copper heat sink is 1.3 times higher than that of the microchannels and 4 times higher than that of the conventional groove fins.

8.4

Conclusions

The following conclusions were drawn from the experimental and numerical investigation on the effective thermal conductivity of lotus copper:

1. The lotus copper exhibited anisotropy for the effective thermal conductivity. The effective thermal conductivity $k_{\text{eff}\perp}$ perpendicular to the pores was lower than that parallel to the pores $k_{\text{eff}\parallel}$ and was 40% of that of the lotus copper material k_s for the case of a porosity of 0.4.
2. Experimental data for $k_{\text{eff}\parallel}$ showed good agreement with the analytical results derived from the assumption that heat flow through the cross-sectional area parallel to the pore axis is proportional to $(1 - \varepsilon)$.
3. Experimental data for $k_{\text{eff}\perp}$ showed good agreement with the analytical results derived from the assumption of orthorhombic symmetry and with the numerical results under a uniform staggered array with a nonuniform pore diameter condition.
4. The effective thermal conductivity perpendicular to the pores of the lotus metal in which pore shape is not necessarily circular and the diameter is not uniform can be predicted within a 10% discrepancy by Behrens' equation as a function of porosity.

From the experimental and analytical investigation of the lotus-type porous copper heat sink, the following conclusions were drawn:

1. The fin efficiency of the lotus-type porous copper fin is verified to be predictable by the straight fin model using the effective thermal conductivity perpendicular to the pore axis and the surface area ratio between the surface area of the lotus copper and straight fin.
2. The heat transfer coefficient based on the base plate area and the pressure drop of the lotus-type copper heat sink can be predicted by using the correlation for circular pipes within an accuracy of $\pm 15\%$ and $\pm 5\%$, respectively.
3. The heat transfer capacity of the lotus-type porous copper fins was very large and was found to be 4 times larger than the conventional groove fins and 1.3 times larger than microchannel heat sink under the same pumping power.

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9

Thermal Characterization of Open-Celled Metal Foams by Direct Simulation*

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9.1

Introduction

Foams and other highly porous cellular solids have many interesting combinations of physical, mechanical, electrical and thermal properties such as high stiffness, flow permeability and thermal and electrical conductivity along with low specific weight. Many common materials are highly porous in nature. Examples of such highly porous natural materials include cork, wood, bones (trabecular and cancellous) and sponges [1–3]. Current state-of-the-art manufacturing methods allow foaming of polymers, most metals and their alloys, ceramics and graphite. Among the available synthetic open porous materials, polymer foams have enjoyed widespread use in many industrial technologies [3]. Recently, open-cell metal foams have been attracting increased attention as multifunctional materials due to their versatility in absorbing sound and energy [2]. Open-cell foams have a random reticulated structure of open polyhedral cells connected by continuous metal ligaments. Due to their highly porous reticulated nature, open-cell foams with negative Poisson's ratio (termed auxetic foams) have been produced by Lakes [4] and by many others [5] from conventional positive Poisson's ratio materials. Depending on the porosity of the cellular materials, a wide range of applications are possible. Figure 9.1 shows the variation of the degree of openness of the foams and their corresponding applications [3].

Open-cell foams have been proposed for many applications such as porous tissue engineering scaffolds [6,7], hydrogen storage technologies [8], thermal control of electronics, catalysis [9], solar energy storage [10], electrochemical cells [11] and others [2,12]. The work described in this chapter is primarily concerned with thermal management applications. With increased heat dissipation requirements for micro-processors [13] and many other electronics systems, demand for the development of compact heat dissipation systems continues to increase. Open-cell materials, owing to their ability to integrate multiple functions, are very attractive as thermal management materials. Many previous investigators have proposed and analyzed metal

* Please find the nomenclature at the end of this chapter.

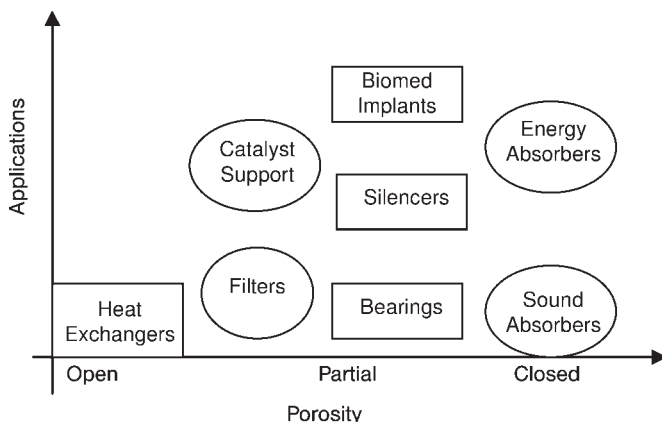


Figure 9.1 Applications of porous cellular materials classified by the type of cellular geometry (adapted from [3]).

foams for possible applications as heat exchangers [14–17], heat sinks [18,19] and heat pipe wicks.

Flows in porous media may be modeled using two major classes of approaches: (a) a macroscopic approach, where volume-averaged semi-empirical equations are used to describe flow characteristics, and (b) a microscopic approach, where small-scale flow details are simulated by considering the specific geometry of the porous medium.

In the first approach, small-scale details are ignored and the information so lost is represented in the governing equations using an engineering model. For instance, the method of volume averaging transforms the effects of the internal geometry of the porous medium to a macroscopic representative elementary volume (REV) [20]. This transformation requires that the thermal interaction between the different phases in the REV be accounted for and modeled. In general, this difficulty is resolved by invoking the thermal equilibrium assumption, i.e. assuming negligible temperature difference (or comparable local temperature gradients) between the solid and fluid phases within the REV. In certain situations this assumption of thermal equilibrium between the solid microstructure and saturating fluid phase is invalid. Such situations include the presence of internal heat generation in one of the phases, heat transfer augmentation (using metal foams and metal fillers) where the thermal diffusivities of the porous matrix and the saturating fluid (e.g. air, water) are very different, and during transient operation in systems with very different response times [18,19]. To account for the local thermal nonequilibrium conditions a two-medium treatment should be used [18,19,21]. The governing energy transport equations are written for the solid (e.g. metal foam) and interstitial material (e.g. air) separately and they are closed (coupled) using an interstitial heat transfer coefficient [18]. Details of the method of volume averaging can be found in [20]. Further discussion of the validity of the local thermal equilibrium assumption may be found in [18,21].

In the second approach, the intricate geometry of the porous structures is accounted for and the transport through these structures computed. The latter approach is computationally expensive if the entire physical domain were to be simulated. Computational time can be reduced by exploiting periodicity when it exists. Resolution of flow and heat transfer at the pore scale is necessary for a number of reasons when modeling metal foams. Detailed modeling of pore-scale heat transfer has been used to yield the effective thermal conductivity of the foam for situations with no flow. Existing models have frequently used idealized (and approximate) geometries assuming one-dimensional conduction heat transfer with a free parameter which is adjusted to match experimental results [22,23]. Another use for pore-scale models is to better characterize the pressure drop and local heat transfer coefficient during flow and convective heat transfer through the foam. Though there have been a few studies which take this approach [24,25], the range of Reynolds numbers considered does not adequately cover metallic foams impregnated with phase change materials (PCMs), where the pore Reynolds numbers are very small ($Re < 1$) [19]. The geometric representation of the foam varies greatly in the literature. Past investigators have represented the open-celled foam structure using: (a) simple cubic unit cells consisting of slender circular cylinders [14], (b) cubic unit cells consisting of square cylinders [26], (c) truncated tetrakai-decahedron unit cells with triangular strands (fibers) [24] and (d) a Weaire–Phelan unit cell [25]. Results from these models have included effective thermal conductivity and pressure drop calculations, but no information has been reported on local heat transfer. The local heat transfer coefficients are very important for closing (coupling) the solid and fluid energy equations in the two-medium volume-averaged models [18,19,21,27]. Also, the unit cell used to predict effective thermal conductivity is frequently different from those used for flow calculations [28]. The effective thermal conductivity, pressure drop and local heat transfer coefficient are obtained here from a consistent direct simulation of the open-cell foam structure.

9.2

Foam Geometry

A three-dimensional periodic module is identified for the direct simulation of open-cell foams. The geometry chosen should be space-filling and should have minimum surface energy. This is required because of the nature of the foaming process. For example, a popular method for foaming metals such as aluminum is by blowing a foaming gas through molten metal with ceramic particles (used for stabilization) from below [2]. The gas bubbles developed are free to move around and pack themselves. The liquid metal accumulates at the interstices between the bubbles. For the process to reach a steady state, the bubbles must attain an equilibrium, i.e. a minimum surface energy state. Once the molten foam is solidified the open-cell foam is rolled into sheets or into any other desired form [2]. The Weaire–Phelan (WP) unit cell (or A15 lattice)

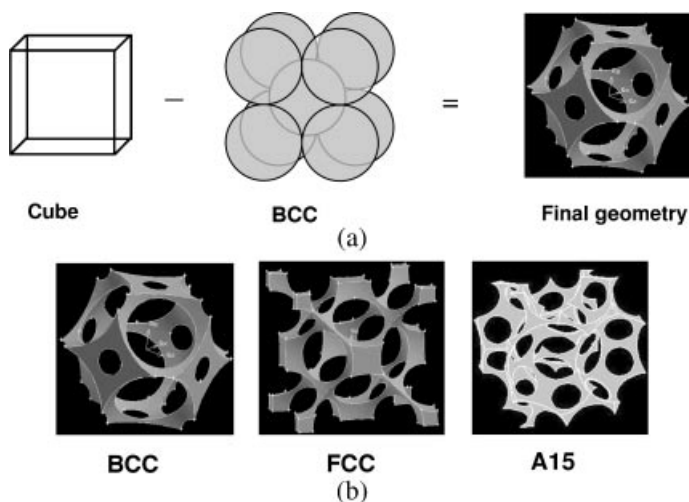


Figure 9.2 (a) Schematic representation of foam geometry creation and (b) sample images of foam geometry created for BCC, FCC, and A15 arrangements of spherical pores.

has the minimum surface area to volume ratio compared to all other space-filling structures [29].

In the present approach for foam geometry creation, the shape of the pore is assumed to be spherical and spheres of equal volume are arranged according to the following three lattice structures: (a) the body-centered cubic (BCC) lattice arrangement for Kelvin's unit cell, (b) the face-centered cubic (FCC) lattice and (c) the A15 lattice, for the WP structure [29,30]. The periodic foam unit cell geometry is obtained by subtracting the unit cell cube from the spheres at the various lattice points as shown in Figure 9.2a. The cross-section of the foam ligaments is a set of convex triangles (plateau borders), all of which meet at symmetric tetrahedral vertices [29]. It may be noted that there is a nonuniform distribution of metal mass along the length of the ligament with more mass accumulating at the vertices (nodes) resulting in a thinning at the center of the ligament as experimentally observed in foam samples by many authors [2,23,28,31]. Figure 9.2b shows some sample open-cell structures.

The distinguishing feature of this direct simulation approach is that (a) the geometry creation is simple, (b) it captures many of the important features of real foams and (c) meshing of the geometry is easier as compared to the approach carried out in [25] for modeling pressure drops. In [25] the foam was represented by an ideal WP unit cell obtained using Surface Evolver, a surface minimization software program [32]. The idealized geometry was exported to a mesh generation program. After a series of post-processing steps on the geometry obtained from Surface Evolver, an unstructured volume mesh was generated for CFD (computational fluid dynamics) calculations.

9.3

Mathematical Modeling

9.3.1

Effective Thermal Conductivity

Consider a module with periodic boundaries separated by a constant translation vector ($\vec{L}$), as shown in Figure 9.3. This module represents one of a series of periodic modules translated by $\vec{L}$ representing the foam. It should be noted that there may be other periodic boundaries in the module, but there is no net inflow through any of these boundaries. The effective thermal conductivity of the foam is computed by considering heat conduction through the solid structure and the fluid in the module, in the absence of convection. Now consider the periodic module as being a part of a sufficiently long physical domain in steady state, with a temperature gradient applied across it in the vector direction $\vec{L}$. The heat transfer rate passing through the module in the direction $\vec{L}$ is constant in each module. Equivalently, each module in the heat flow direction experiences an equal temperature drop ΔT . This condition allows the imposition of a *jump-periodic* condition on temperature, analogous to the fully developed heat-flux condition for duct flows. The jump-periodic condition implies that the temperatures in adjacent modules are related by

$$\nabla T(\vec{r}) = \nabla T(\vec{r} + \vec{L}) = \nabla T(\vec{r} - \vec{L}) \quad (9.1)$$

where $\vec{r}$ represents the position vector under consideration. For periodic boundaries across which there is no net flow, the temperature T is assumed periodic.

Within each module, the heat conduction equation may be written in the solid and fluid domains as

$$\frac{\partial}{\partial x_i} \left(k_s \frac{\partial T_s}{\partial x_i} \right) = 0$$

$$\frac{\partial}{\partial x_i} \left(k_f \frac{\partial T_f}{\partial x_i} \right) = 0$$

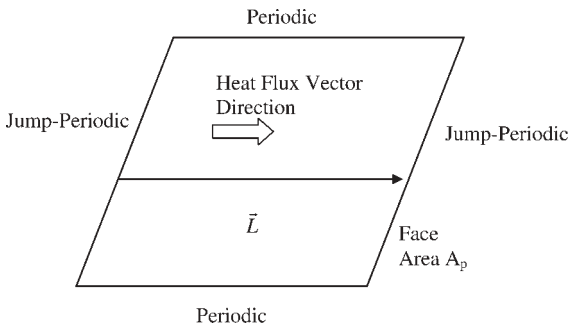


Figure 9.3 Nomenclature for jump-periodic boundary condition for computing effective thermal conductivity.

where T_s and T_f are the temperatures of the solid and fluid respectively. At the fluid/solid interface, the two temperature fields are related by

$$-k_s \frac{\partial T_s}{\partial n} \Big|_{\text{interface}} = -k_f \frac{\partial T_f}{\partial n} \Big|_{\text{interface}} ; \quad T_s|_{\text{interface}} = T_f|_{\text{interface}}$$

where n represents the direction normal to the fluid/solid interface.

The unstructured finite volume method described in [33] is used for the solution of the above equations and boundary conditions. The numerical implementation of the periodic condition described by Eq. (9.1) in the unstructured finite volume framework is described in [33]. The jump-periodic condition is implemented by choosing an arbitrary temperature drop ΔT across the module in the heat flow direction and finding the resulting heat transfer rate at the jump-periodic boundaries from the simulation results. The effective thermal conductivity of the module is then given by the expression

$$k_{\text{eff}} = \frac{-\int_{A_p} \mathbf{J} \cdot d\mathbf{A}}{(\Delta T A_p / L)} \quad (9.2)$$

where $\mathbf{J}$ is the diffusion flux vector at the jump-periodic face obtained from the simulation, $d\mathbf{A}$ is the outward pointing elemental face area vector on the jump-periodic face and A_p is the area of the jump-periodic face normal to $\vec{L}$. Computations are performed using a modified version of the commercial code FLUENT [36]. It is noted that conduction through the solid foam and the fluid are considered for the calculation of the effective thermal conductivity of the module.

9.3.2

Computation of Flow and Heat Transfer Through Foam

Similar to the effective thermal conductivity calculation, the computation of the pressure drop and heat transfer coefficient for flow through the foam also considers a periodic module containing the foam unit cell, but does not consider the solid region. Instead, the governing flow and energy equations are solved in the fluid region, with no-slip and given-heat flux boundary conditions imposed at the fluid/solid interface. Details are given below.

9.3.2.1 Flow and Temperature Periodicity

A schematic illustration of a periodic foam geometry is shown in Figure 9.4. For periodic boundaries, according to [34], the following relationship holds for the velocity and the pressure at any position $\vec{r}$:

$$u_i(\vec{r}) = u_i(\vec{r} + \vec{L}) = u_i(\vec{r} + 2\vec{L}) = \dots$$

$$P(\vec{r}) - P(\vec{r} + \vec{L}) = P(\vec{r} + \vec{L}) - P(\vec{r} + 2\vec{L}) = \dots$$

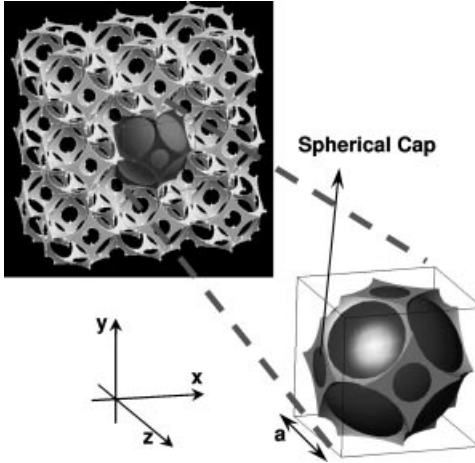


Figure 9.4 Schematic of a periodic BCC unit cell.

For periodic flows, the pressure gradient can be divided into two components – the gradient of the periodic component, $\partial \bar{p} / \partial x_i$, and the gradient of a linearly varying component, $(\partial \bar{p} / \partial x_i) \vec{e}_L$:

$$\frac{\partial P}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_i} \vec{e}_{L,i} + \frac{\partial \hat{p}}{\partial x_i}$$

where $e_{L,i}$ is the i th component of the unit vector $\vec{e}_L$ in the direction $\vec{L}$.

For given heat-flux boundary conditions, the shape of the temperature field becomes constant from module to module. Consequently, the periodic condition for the temperature is given by

$$T(\vec{r}) - T_b(\vec{r}) = T(\vec{r} + \vec{L}) - T_b(\vec{r} + \vec{L}) = T(\vec{r} + 2\vec{L}) - T_b(\vec{r} + 2\vec{L}) = \dots$$

Here the bulk temperature T_b is defined as

$$\frac{\iint_A |u_i e_{L,i}| T \, dA}{\iint_A |u_i e_{L,i}| \, dA} = T_b$$

where A is the area of cross-section.

9.3.2.2 Governing Equations

The governing flow and heat transfer equations for periodic, fully developed, incompressible, steady flow of a Newtonian fluid are [34,35]

$$\frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad (9.3)$$

$$\frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial u_i}{\partial x_j} \right)_i - \frac{\partial \bar{p}}{\partial x_i} e_{L,i} \quad (9.4)$$

$$\frac{\partial}{\partial x_i} (\rho C_p)_f u_i T_f = \frac{\partial}{\partial x_i} \left(k_f \frac{\partial T_f}{\partial x_i} \right) \quad (9.5)$$

The above equations assume that the flow is thermally and hydrodynamically fully developed. In Eq. (9.4), the terms involving $\partial^2/\partial x^2$ have been included to account for the large local streamwise gradients that may occur in periodically fully developed flows. The quantity $\partial \bar{p}/\partial x_i$ in Eq. (9.4) is assigned *a priori*, and controls the mass flow rate through the module, and hence the pore Reynolds number. In order to sustain periodicity, all fluid properties are assumed to be independent of temperature. It should be noted that on the solid bounding walls a no-slip boundary condition is imposed for the velocities and a constant heat flux is specified for the energy equation. Details of the mathematical model are available in [34]. An extensive treatment of the numerical method for the periodic flow and heat transfer on unstructured meshes along with the implementation is given in [35].

9.3.2.3 Computational Details

The governing flow and heat transfer equations for periodic fully developed, incompressible, steady flow of a Newtonian fluid are solved using the commercial software FLUENT [36]. The periodic unit cell geometry was created using the commercial software GAMBIT [37]. The geometry was meshed using hybrid (tetrahedral and hexagonal) elements in GAMBIT by specifying the minimum edge length. The mesh so created was exported to the commercial code FLUENT for flow simulations. A second-order upwind scheme was used for the flow and heat transfer calculations. A co-located pressure-velocity formulation in conjunction with the SIMPLE algorithm was used for obtaining the velocity fields, and the linearized systems of equations are solved using an algebraic multigrid algorithm. Details of the numerical method may be found in [38]. The calculations were terminated when the (scaled) residual [36] had dropped below 10^{-7} for all governing equations.

Grid independence of the solution for the meshes used in the present simulations was established. A pore Reynolds number of 20, a Prandtl number of 0.71 and a porosity of 0.965 were used for this set of calculations. Grid sensitivity was tested on three different grids: grid 1 (106 520 cells), grid 2 (188 885 cells) and grid 3 (383 230 cells). For grid 1, deviations of 2.6% and 0.5% in the friction factor and Nusselt number were found with respect to grid 3. For grid 2, the corresponding deviations with respect to grid 3 were 0.9% and 0.4%. The calculations reported here were therefore performed on grid 2.

9.4

Results and Discussion

First, the effective thermal conductivity, friction factor and Nusselt number results for the BCC model are discussed. Then, the effects of choosing other periodic unit cell geometries to represent open-cell foams are presented.

9.4.1

Direct Simulations of Foams: BCC Model

The expression for the porosity of the periodic module and the fluid inlet area of the periodic face can be obtained by accounting for the overlapping sphere volumes and circle areas, respectively. The intersection volume (lens volume) between two overlapping spheres is given by the relation

$$V_{\text{int}} = \frac{\pi}{12} (4R + s)(2R - s)^2 \quad (9.6)$$

where s is the center-to-center distance between the in-line spheres and R is the radius of the sphere. The body-centered sphere intersects with eight spheres on the vertices of the cube and hence the volume of the sphere at the body center of the cube is

$$V'_{\text{bc}} = \frac{4\pi}{3} R^3 - 8 \left[\frac{V_{\text{int}}}{2} \right] \quad (9.7)$$

Besides the sphere at the body center, one additional sphere volume contributed by the 8 segments of the sphere at the vertices. Hence the total sphere volume not accounting for the spherical caps (see Figure 9.4) at the intersection between the face of the cube (plane) and the spheres is twice the V'_{bc} given in Eq. (9.7). The volume occupied by the spherical cap (the protruding volume from the unit cube for sphere diameter larger than length of the cube) due to a sphere intersecting a plane is given by the expression

$$V'_{\text{sc}} = \frac{\pi}{3} \left(R - \frac{s}{2} \right)^2 \left(2R + \frac{s}{2} \right)$$

There are six spherical caps for the six corresponding faces of the cube and hence the volume of the fluid space in the cube is given by the expression

$$V'_f = 2 \left[\frac{4\pi}{3} R^3 - \frac{\pi}{3} (4R + s)(2R - s)^2 - 2\pi \left(R - \frac{a}{2} \right)^2 \left(2R + \frac{a}{2} \right) \right]$$

and the porosity is given by the relation

$$\varepsilon = \frac{V'_f}{V} = \frac{2 \left[\frac{4\pi}{3} R^3 - \frac{\pi}{3} (4R + s)(2R - s)^2 - 2\pi \left(R - \frac{a}{2} \right)^2 \left(2R + \frac{a}{2} \right) \right]}{a^3} \quad (9.8)$$

Similarly, the inlet face area for the fluid can be obtained by subtracting the circle area and the intersection area between the sphere and the plane from the face area.

The inlet face area is given by the expression

$$A_{\text{in,f}} = \pi R^2 - 2 \left[2R^2 \cos^{-1} \left(\frac{s}{2R} \right) - \frac{1}{2} s \sqrt{4R^2 - s^2} \right] + \pi \left(\frac{4R^2 - a^2}{4} \right) \quad (9.9)$$

where a is the length of the side of the unit cell, and is equal to the magnitude of the periodic displacement vector $\vec{L}$. It should be noted that the center-to-center distance ($\sqrt{3}a/2$) for the volume (porosity) calculation is different from the center-to-center distance ($a/2$) for the area calculation. An effective pore diameter was extracted by setting Eq. (9.9) equal to the area of an equivalent circle. It should be noted that exactly at a sphere radius of 0.5, the BCC structure ceases to be a completely open structure, and the corresponding porosity at this condition is 0.94. The implication of this porosity value on model fidelity is discussed later.

9.4.1.1 Effective Thermal Conductivity

Lemlich Theory Lemlich [39] developed a theory to predict the electrical conductivity of a polyhedral liquid foam of high porosity. The electrical conduction is viewed as occurring only through the plateau border (ligament in the case of solid foams) along its axis, and not through its periphery. He found that the effective electrical conductivity of the foam was related to the electrical conductivity of the liquid through the following relation:

$$\sigma_{\text{eff}} = \sigma_l \frac{(1 - \varepsilon)}{3} \quad (9.10)$$

This expression can be used for the effective thermal conductivity of the solid foam by exploiting the analogy between Ohm's law and Fourier's law, so that

$$k_{\text{eff}} = k_s \frac{(1 - \varepsilon)}{3} \quad (9.11)$$

Figures 9.5a and b show the predicted effective thermal conductivity from the simulations as a function of porosity for an open-cell foam saturated with air and water, respectively. Also plotted in Figure 9.5 are measured experimental values [23,40] and results from semi-empirical models in the literature [22,23]. It can be seen from Figure 9.5 that the present model compares well with the experiments (both air and water) and the other models for porosities above 0.94. The foam geometry ceases to be “open”-celled for porosities below 0.94, as shown in Figure 9.6. It may be recalled that the models of Boomsma and Poulikakos [22], Calmidi and Mahajan [23] and Bhattacharya *et al.* [28] employ an adjustable free parameter to match the experiments of Calmidi and Mahajan [23]. The computations in this work employ no such adjustable parameter; here, the attempt is to compute directly the effective conductivity from a detailed description of the foam geometry. However, deviations from experimental data reflect the inadequacy of the present geometric model at lower porosities.

The Lemlich theory predicts the thermal conductivity values well when the interstitial fluid is air (Figure 9.5a), but is less successful with water saturation (Figure 9.5b). This deviation for water is primarily due to the assumption of

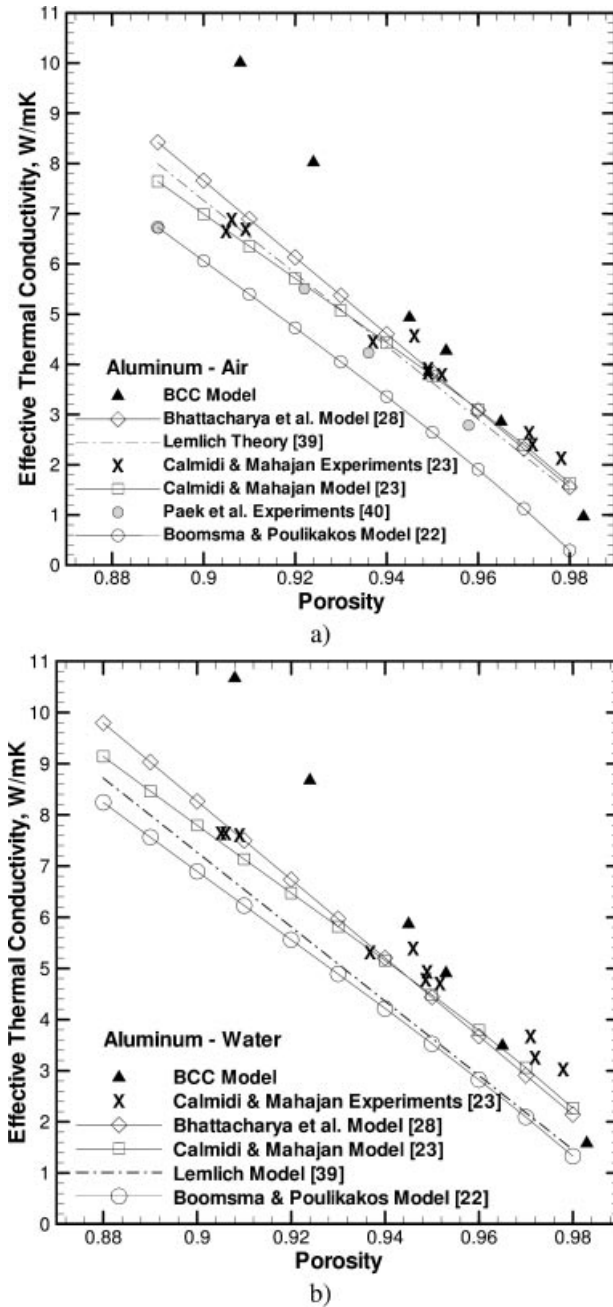


Figure 9.5 Effective thermal conductivity as a function of porosity for aluminum foam saturated with (a) air and (b) water. The thermal conductivity values used for aluminum, air and water are 218, 0.0265 and $0.613 \text{ W m}^{-1} \text{ K}^{-1}$, respectively [22].

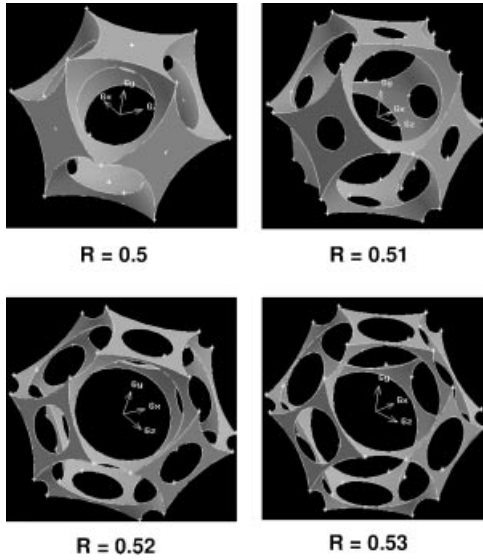


Figure 9.6 Sample images of the evolution of open-cell geometry as function of sphere radius.

negligible heat exchange to the interstitial fluid in the theory, and also due to the ignored contribution of nodal resistance at the tetrahedral vertices. In the case of water (whose thermal conductivity is an order of magnitude higher than that of air) the heat exchange between the foam ligament and interstitial fluid is more significant. Thus, though Eq. (9.11) is an approximation and some departure from experiment is expected, it may be used for reasonably satisfactory order-of-magnitude estimates of effective thermal conductivity of open-cell foams.

9.4.1.2 Pressure Drop and Heat Transfer Coefficient

For the calculations presented in this section, a constant heat-flux boundary condition is imposed on the ligament walls. Hence, conduction through the ligaments of the foam is neglected. The streamwise diffusion term is retained in the momentum and energy equations which govern the generalized fully developed regime [34].

For a fluid flowing through a porous medium, boundary layer growth is significant only over an axial length of order $(\rho K u_D)/\mu$ where u_D is $(K/\mu)dP/dx$. Similarly, the thermal boundary layer development length is on the order of $K u_D/\alpha$. The flow penetration is usually of the order of $\sqrt{K}$, the characteristic length scale. Unlike packed beds of spheres, the porosity and permeability for open-cell foams are constant even close to the solid boundary, i.e. the porosity does not change near the boundaries. In this section, a representative case of porosity of 0.965 with air being the interstitial fluid is discussed first. The predicted variation of friction factor and local Nusselt number are subsequently considered.

Figure 9.7 shows the predicted dimensionless u -velocity field normalized using the mean velocity for a porosity of 0.965. The Reynolds number based on the

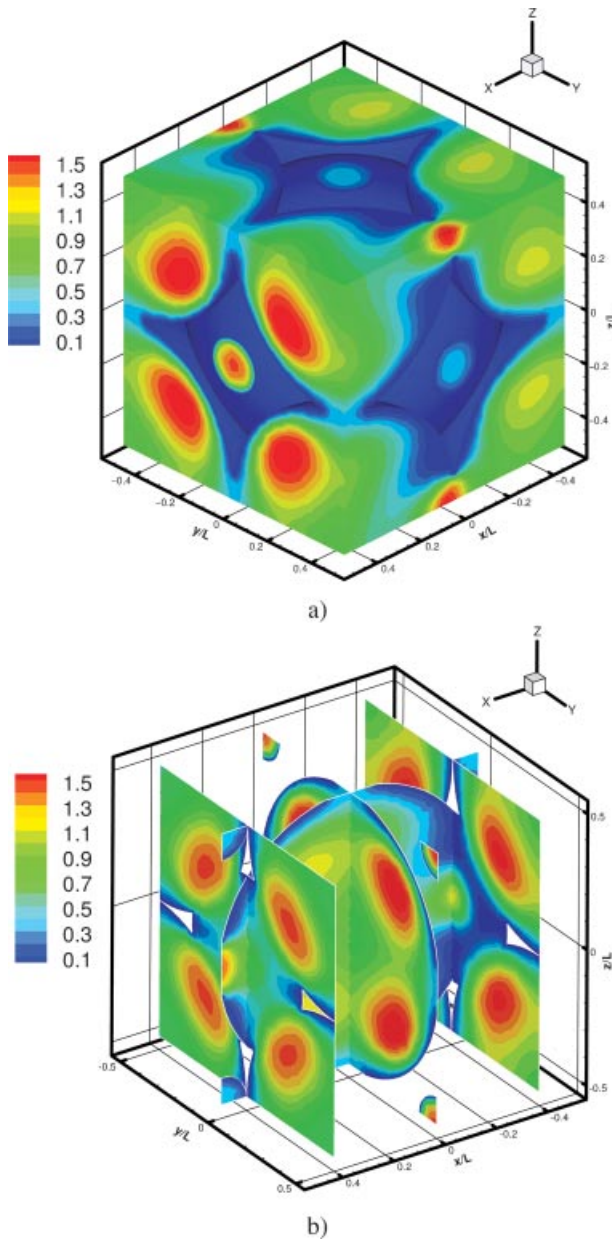


Figure 9.7 Predicted results for (a) dimensionless velocity field and (b) dimensionless velocity field at different locations ($x/L = -0.4, 0.0, 0.4$ and $y/L = 0$).

effective diameter of the pore is 50 and the Prandtl number is 0.7. The effective diameter for all the computations is obtained by setting Eq. (9.9) equal to the area of a circle and backing out the effective diameter. Figure 9.7b shows the dimensionless velocity field on slices at discrete locations along the axial direction of flow. Also plotted in Figure 9.7b is the velocity field at $y/L = 0$ to illustrate the axial flow. The flow enters at the periodic inlet, $x/L = -0.5$. Periodic conditions are specified on all the boundary faces of the cubic unit cell. The solid boundaries are demarcated in white in the figure. From Figure 9.7 the boundary layer development at the solid boundaries can be seen. Due to the resistance offered by the foam ligaments, the mean velocities are higher in some regions. Figure 9.8 shows the dimensionless temperature distribution, $(T - T_b)/(\bar{T}_s - T_b)$, in the fluid for a porosity of 0.965. As expected, the dimensionless temperature at the periodic inlet is low and thermal boundary layers can be clearly seen in Figure 9.8b. For $Pe > 1$, thermal dispersion effects become important [41,42] and should be included in volume averaged models. They may be deduced from unit cell models such as those developed here using methods described in [43].

Figure 9.9 shows the predicted normalized permeability of the foam as a function of porosity. Also shown are the experimental measurements from Bhattacharya *et al.* [28]. The permeability is normalized with the mean pore diameter of the open cell. The permeability is calculated from Darcy's law, $K = -(\mu u_{\text{mean}})(\partial \bar{p}/\partial x_i)$, where u_{mean} is obtained from the specified periodic inlet mass flow rate and using Eq. (9.9). The pressure drop is obtained as an output from the simulations. The reported permeability values are averaged values over a Reynolds number range of 1 to 10, i.e. in the linear Darcy regime.

Friction factors for the different cases considered are shown in Figure 9.10 for porosities greater than 0.94. Also plotted in Figure 9.10 are predictions from the experimental correlations of Paek *et al.* [40] and Vafai and Tien [44]. The friction factor is defined as

$$f = \frac{\left(-\frac{\partial \bar{p}}{\partial x_i}\right) \sqrt{K}}{\rho u_{\text{mean}}^2} \quad (9.12)$$

and in the Darcy regime, the friction factor (f) scales as the inverse of the modified Reynolds number based on the flow penetration length ($f = 1/Re_K$). From Figure 9.10 it can be seen that for the porosity and modified Reynolds number ($Re_K \approx 1-10$) ranges considered in this study, the flow of both air and water through the foam is still in the Darcy regime. Deviations from $1/Re_K$ behavior were observed near a modified Reynolds number of approximately 20 for both air and water.

The Nusselt number for the foam was also calculated for the different cases considered and is defined as

$$Nu = \frac{hD}{k_f} = \frac{q''D}{k_f(\bar{T}_s - T_b)} \quad (9.13)$$

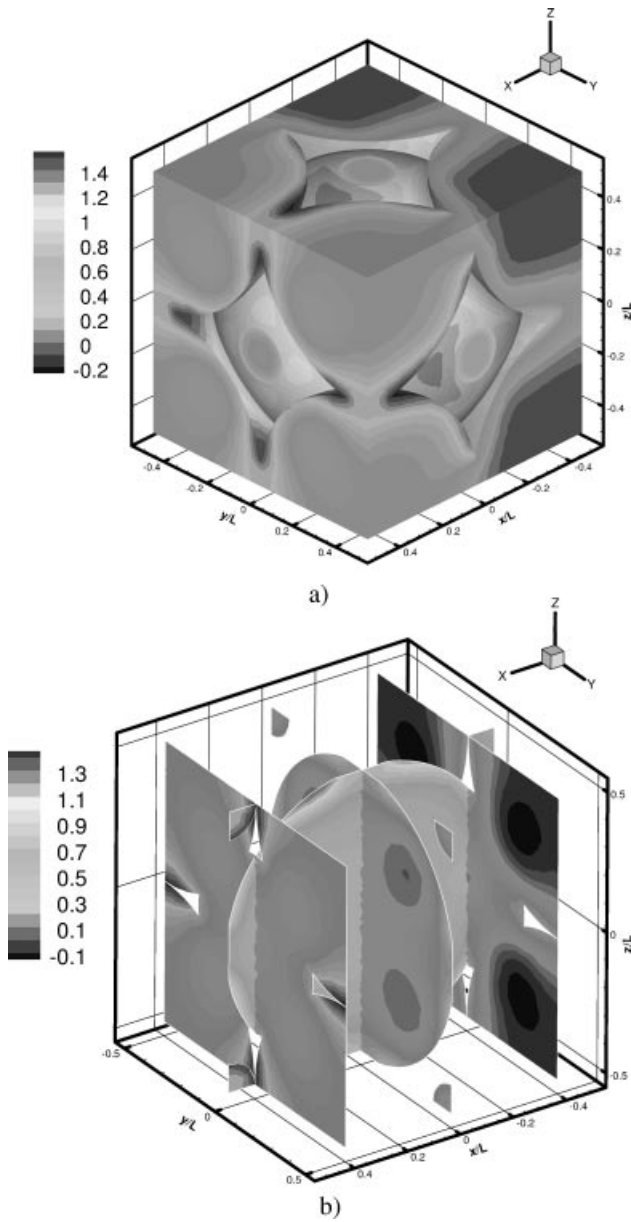


Figure 9.8 Predicted results for (a) dimensionless temperature field and (b) dimensionless temperature maps at different locations ($x/L = -0.4, 0$ and 0.4 and $y/L = 0$).

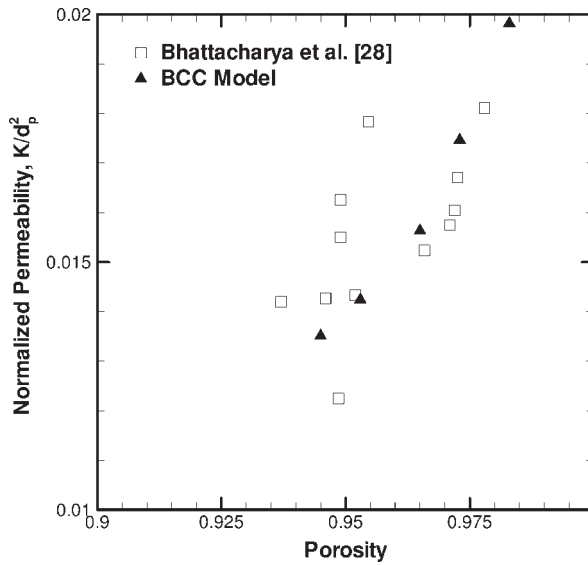


Figure 9.9 Predicted normalized permeability of the foam as a function of the porosity of the foam. Also plotted are experimental data points from Bhattacharya *et al.* [28].

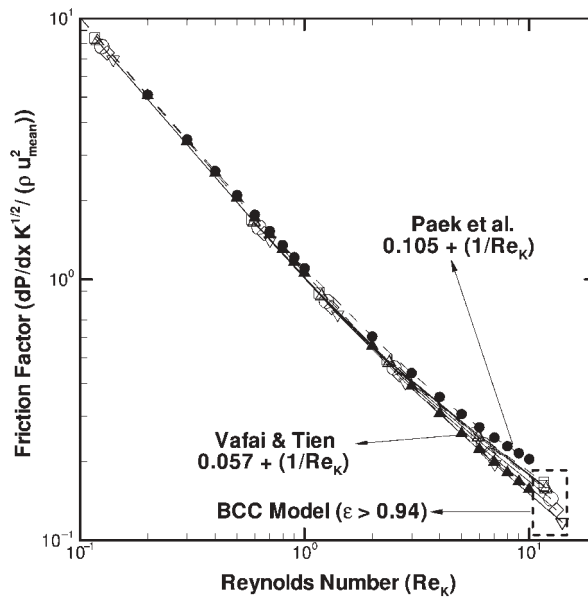


Figure 9.10 Predicted friction factor as a function of Reynolds number based on the flow penetration length ($\sqrt{K}$). Also plotted are experimental correlations from Paek *et al.* [40] and Vafai and Tien [44]. Symbols are defined in Figure 9.10.

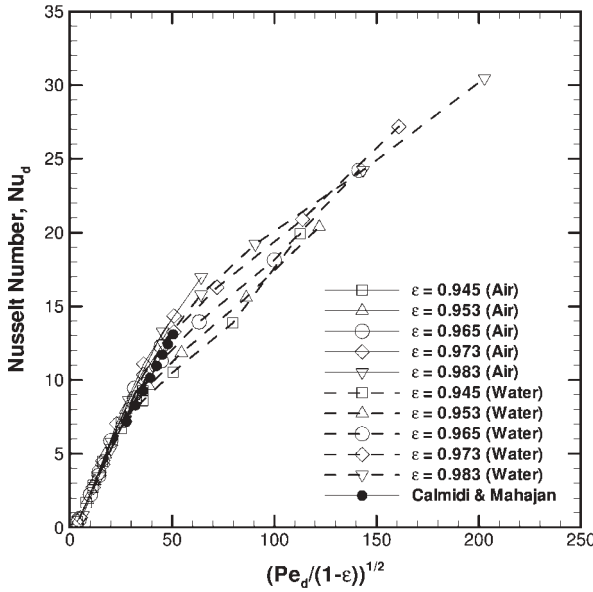


Figure 9.11 Predicted Nusselt number based on effective diameter of the pore as a function of the square root of the Peclet number ($Re_d Pr / (1 - \epsilon)$). Also plotted is the correlation from Calmidi and Mahajan [45].

where $\bar{T}_s$ is the averaged temperature of the foam. Figure 9.11 shows the predicted Nusselt number as a function of the square root of the Peclet number. This scale is readily obtained by balancing the convective and axial diffusive fluxes. Also plotted in Figure 9.11 are values from the correlation of Calmidi and Mahajan computed for air and for a porosity of 0.973 [45]. While their original correlation was based on the fiber diameter, it is re-scaled here in terms of mean pore diameter, with 0.00402 m and 0.0005 m as the fiber and pore diameters, respectively [45]. The curves for air and water are seen to each collapse to a single line with a unique slope for $Pe_d < 30$.

9.4.2

Direct Simulations of Foams: Effect of Unit Cell Structure

In this section, we consider alternative geometric representations of the foam geometry. We use the same methodology for geometry creation as discussed in the previous section. The shape of the pore is assumed to be spherical and spheres of equal volume are arranged according to the following two lattice structures: (a) FCC and (b) A15 lattice, a geometry similar to the WP structure [29,30]. The periodic foam unit cell geometry is obtained by subtracting the unit cell cube from the spheres at the various lattice points as shown in Figure 9.2.

9.4.2.1 Effective Thermal Conductivity

The numerical results for effective thermal conductivity for an aluminum–air system are considered first. The effective thermal conductivity is computed by numerically solving the conduction heat transfer through both the metal foam and the interstitial air in a single periodic module as discussed previously.

Figure 9.12 shows the calculated effective thermal conductivity for an aluminum foam–air system as a function of foam porosity. Also plotted in Figure 9.12 are the predictions from the available semi-empirical models, and experimental measurements from the literature. Available experimental effective thermal conductivity measurements for foams cover a porosity range of $0.89 < \varepsilon < 0.98$. Paek *et al.* [40] and Calmidi and Mahajan [23] reported an experimental uncertainty of 12% and 3.6% for the effective thermal conductivity measurements, respectively. It should be noted that the BCC, FCC and A15 models in the present work do not employ any arbitrary parameter to match the experiments. Also plotted is the theoretical result from Lemlich's original work discussed previously (Eq. (9.11)). It can be inferred from Figure 9.12 that both A15 and BCC models compare well with the existing literature for high porosities. The BCC model, as discussed previously, deviates from experiments at a porosity of 0.94 because the foam geometry ceases to be open-celled, and there is an accumulation of metal mass at the nodes. The predictions of the A15 model match experiments at lower porosities down

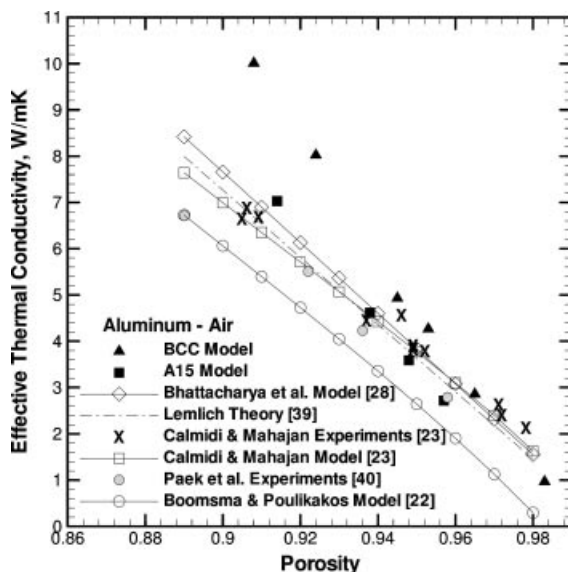


Figure 9.12 Predicted effective thermal conductivity of an aluminum foam–air system for a range of porosities. Also plotted are available semi-empirical models and experimental measurements.

to $\varepsilon > 0.9$. However, no experimental data are available for porosities below 0.9, and computations below this limit cannot be validated. In Figure 9.12, the predictions from the FCC model are not plotted because the model under-predicted the experimental results by a factor of approximately 2.5.

9.4.2.2 Pressure Drop and Nusselt Number

We now consider predictions of the pressure drop and Nusselt number for the FCC and A15 lattice models and compare them with the predictions of the BCC model. All other modeling assumptions are the same as those described for the BCC model. Figure 9.13 shows the results for the friction factor calculated for an aluminum foam–air system from the numerical simulations based on the FCC and A15 periodic modules. Also plotted are the experimental correlations [40,44]. Paek *et al.* [40] reported the repeatability error for the measurement of pressure drop to be 3% for foam samples of porosity $0.89 < \varepsilon < 0.97$. The porosity range considered by Vafai and Tien [44] was $0.94 < \varepsilon < 0.97$. The permeability of the foam was calculated using the expression $K = -(\mu u_{\text{mean}})(\partial \bar{p} / \partial x_i)$, where u_{mean} was obtained for specified inlet mass flow rate in the Darcy regime ($Re < 10$). The friction factor shown in Figure 9.13 is defined in Eq. (9.12). The predicted friction factors from all the three models (BCC, FCC and A15) compare well with the experimental correlations for porosities $\varepsilon > 0.88$, while deviations for both the FCC and A15 structures are observed for porosities $\varepsilon < 0.88$. The FCC model over-predicts the friction factor compared to the A15 model.

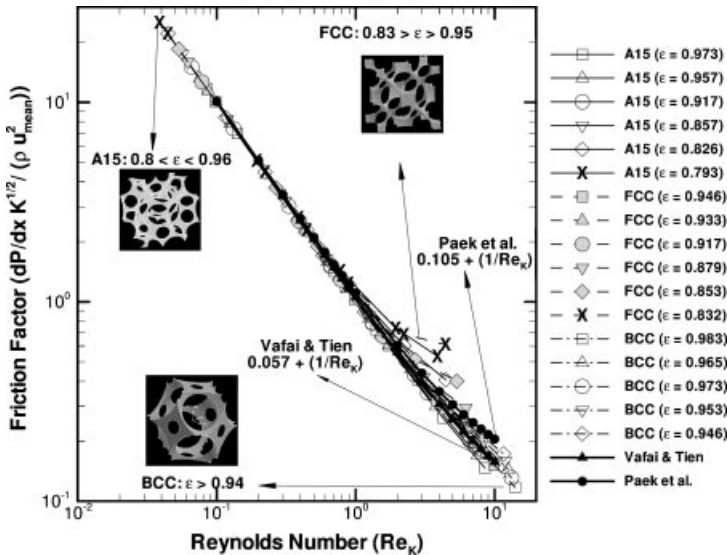


Figure 9.13 Predicted friction factor as a function of modified Reynolds number ($Re_K = Re_d (\sqrt{K}/D)$). Also, experimental correlations from [40] and [44] are plotted.

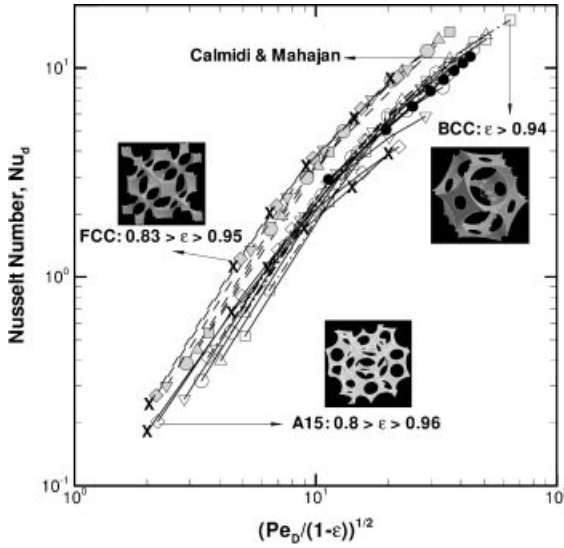


Figure 9.14 Predicted Nusselt number as a function of square root of Peclet number. Symbols as in Figure 9.13.

In Figure 9.14, the predicted local Nusselt number for the FCC and A15 lattices is plotted as a function of $[Pe_D/(1 - \epsilon)]^{1/2}$, where the modified Peclet number (Pe_D) is $Re_d Pr$. This x-axis scale is obtained by balancing the convective and axial diffusive fluxes. It is noted that predictions from the A15 model compare well with those from the BCC model for $\epsilon > 0.86$ and with the experimental correlation [45]. For lower porosities (< 0.86), the local Nusselt number based on the permeability decreases due to the decrease in permeability of the porous medium.

9.5 Conclusion

This work presents an approach for the modeling of open-cell foam geometries for porosities $\epsilon > 0.8$. The distinguishing feature of this approach is that no adjustable geometric parameters were used to match the experiments, unlike in previous published work. The BCC, FCC and A15 unit cell models are shown to predict friction factor and Nusselt number values which are in good agreement with available experimental and semi-analytical results.

The BCC and A15 models also predict thermal conductivity reasonably well. The predictions from the A15 model compare well with the available experimental thermal conductivity measurements ($\epsilon > 0.89$) and with BCC model predictions; the FCC model predictions for effective thermal conductivity showed greater deviations from the measurements. Based on the results, there is a clear need for experimental results at foam porosities below 0.89. For convective flow calculations, the

predicted friction factor and local Nusselt number from both FCC and A15 models compare well with the BCC model and with available experimental results for $\varepsilon > 0.86$.

The accuracy of the pressure drop and Nusselt number predictions depends on how well the unit cell representation captures the surface-to-volume ratio of the real foam. On the other hand, the effective thermal conductivity depends strongly on capturing the ligament resistance correctly, and would require an accurate representation of the ligament cross-sectional area-to-length ratio. An evaluation of unit cell models along these lines would benefit from the characterization of actual foams for a range of porosities and manufacturing techniques.

Nomenclature

a	edge length of the unit cell, m
A	area, m^2
C_p	specific heat capacity, $\text{J kg}^{-1} \text{K}^{-1}$
d	diameter of the pore, m
Da	Darcy number
f	friction factor
h	heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
J	diffusion flux vector, W m^{-2}
K	permeability, m^2
k	thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
L	length of the periodic module, m
Nu	Nusselt number
q''	heat flux, W m^{-2}
Pe	Peclet number
Pr	Prandtl number
R	radius of the pore, m
Re	Reynolds number
s	center-to-center distance, m
T	temperature, K
t	time, s
u, v, w	velocities along x, y, z directions, m s^{-1}
V	volume, m^3
x, y, z	Cartesian coordinates

Greek Symbols

α	thermal diffusivity, $\text{m}^2 \text{s}^{-1}$
ε	porosity
μ	dynamic viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
ρ	density, kg m^{-3}

Superscripts

– average or mean

Subscripts

b bulk
bc body center
D Darcian
eff effective
f fluid
in inlet
int intersection
K permeability
s solid
sa surface area
sc spherical cap

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10

Heat Transfer in Open-Cell Metal Foams Subjected to Oscillating Flow*

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10.1

Introduction

An open-cell metal foam is a porous medium which possesses a true solid skeletal structure. The fully interconnected pore and ligament structures within the foam provide extremely large fluid-to-solid contact surface area and tortuous coolant flow paths which increase dramatically the overall heat transfer rate. The large specific surface area, low density and open-cell nature of metal foams offer a combination of properties ideally suited for high heat flux applications where conventional materials and products are not adequate. An oscillating flow is a periodic flow which reverses its direction alternately in a complete motion cycle. It occurs in many reciprocating motion machines such as internal combustion engines, Stirling cycle engines and plus tube cryocoolers. The periodic reversed flow direction in oscillating flow provides two thermal entrances in the test section, which differs from unidirectional flows and affords efficient cooling effects. Research into the application of oscillating flow in open-cell metal foams will be presented in this chapter.

For the sake of clarity, the contents in this chapter are compartmentalized into three major sections which will be discussed separately. The first section deals with critical properties of open-cell foams and the governing similarity parameters for oscillatory flow through open-cell metal foams. Major findings concerning the heat transfer characteristics of oscillating flow through open-cell foams will also be discussed. Finally, comparison of open-cell metal foams under different flow conditions for thermal management applications will be made. In addition, significant findings and major results related to this topic are summarized in the concluding section. Before the major discussions, a brief literature review of research on the heat transfer phenomena in porous materials will be presented.

* Please find the nomenclature at the end of this chapter.

10.1.1

Fluid Flow and Heat Transfer in Open-Cell Foams

The fundamental theory of fluid flow through permeable media was first proposed by Henry Darcy in 1856. He measured the flow rate for a certain volume of water through a column filled with sand and established an equation to estimate the volumetric flow rate for a steady flow. Dupuit extended Darcy's equation in 1863 by considering more parameters such as the permeability and inertial coefficient of the porous medium, which can be represented by the equation

$$0 = \frac{\Delta P}{\Delta L} - \frac{\mu}{K} u - c \rho_f u^2 \quad (10.1)$$

where $\Delta P/\Delta L$, μ , ρ_f and u are the pressure drop per unit length, viscosity, density and velocity of fluid flow, respectively. K and c are the permeability and form coefficient of porous media. Equation (10.1) provides a global balance of forces acting on a finite fully saturated permeable volume with steady flow of an incompressible fluid. By investigating the effect of fluid viscous shear stress in porous media, Brinkman [1] obtained an extended equation to describe steady flow through porous media given by

$$0 = -\nabla(\phi P') + \mu_e \nabla^2 \mathbf{u}' - \frac{\mu}{K} \phi \mathbf{u}' + c \rho_f \phi^2 |\mathbf{u}'| \mathbf{u}' \quad (10.2)$$

where ϕ is the surface porosity determined by the areas occupied by the fluid and solid, respectively; $\mathbf{u}$ is the velocity vector and μ_e is the effective fluid viscosity which is a function of the fluid viscosity and the geometry of the permeable medium. In the last two decades, many investigations were performed to study the momentum behavior of fluid flow in porous media. Vafai and Tien [2] presented a formal derivation of a general equation for fluid flow through an isotropic, rigid and homogeneous porous medium. Using the volume averaging technique, Hsu and Cheng [3] obtained the final equivalent equation for incompressible fluid through porous media by considering the effective viscosity term, which is represented by

$$\rho_f \left[\frac{\partial \mathbf{u}'}{\partial t} + (\mathbf{u}' \cdot \nabla) \mathbf{u}' \right] = -\nabla(\varepsilon P') + \mu_e \nabla^2 \mathbf{u}' - \frac{\mu}{K} \varepsilon \mathbf{u}' + \frac{F}{\sqrt{K}} \rho_f \varepsilon^2 |\mathbf{u}'| \mathbf{u}' \quad (10.3)$$

where ε and F are the porosity and inertial coefficient of porous medium, respectively. The last two terms of Eq. (10.3) represent the lumped viscous and the lumped form effects within the permeable medium, respectively. Related studies on the fundamental theory of flow through permeable media have been reported by various authors [4–8]. In addition, comprehensive reviews of research carried out on the fluid dynamics in porous media have been presented [9,10].

Based on the understanding of fluid flow through porous media, convective heat transfer in porous media has been investigated extensively. Fundamental studies of heat transfer in porous media have been reported [11–14]. It is recognized that by

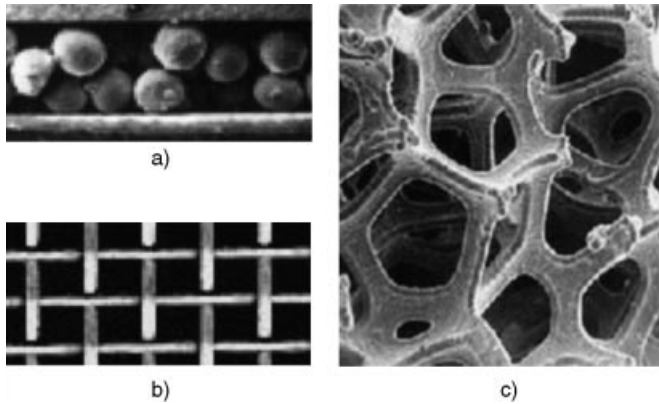


Figure 10.1 Typical structures of (a) particles inserted bed, (b) wire screen and (c) open-cell foam [64].

using porous media, heat transfer can be enhanced substantially due to the increased contact surface area between the porous media and coolant. Porous media have been successfully applied to the cooling of microelectronic chips [15–19], aerospace thermal protective components [20] and high-power laser equipment [21,22]. As compared with a porous channel packed with metal particles, spheres or woven screens, the open-cell foam is a novel type of porous medium. Close-up views of the typical structure for different types of porous media are shown in Figure 10.1. Figures 10.1a and b present the structures for particle-inserted bed and woven screen, respectively. It is observed from Figure 10.1c that the resulting open-cell foam has a reticulated structure of open, shaped cells connected by continuous solid metal ligaments. The open-cell foam with fully interconnected structure, low thermal inertia, high surface area to volume and permeability lends itself to many applications, especially in heat transfer enhancement.

Studies of heat transfer in porous media show that heat transfer characteristics are influenced significantly by material properties such as the geometrical and thermal specifications. The open-cell metal foam has the desirable qualities for heat transfer enhancement, i.e. large specific solid–fluid interface surface area and tortuous fluid paths to promote fluid mixing. Highly conductive metal foams with large porosity and permeability have attracted much attention due to the local thermal dispersion caused by eddies inside the metal foam. Lu *et al.* [23] investigated analytically the heat transfer efficiency in aluminum foams and concluded that the advantage of using a honeycomb structure is that high heat transfer performance can be achieved with relatively small pressure drop. Calmidi and Mahajan [24] studied the effective thermal conductivity of high-porosity fibrous metal foams. Their results showed that the overall effective thermal conductivity of the fluid system could be dramatically increased by metal foams made of aluminum and copper. Noting the influence of the structure on the thermal conductivity of the metal foam matrix, Boomsma and Poulikakos [25] developed a geometrical effective thermal conductivity model of a

saturated open-cell metal foam based on the idealized three-dimensional cell geometry of a foam with a tetrakaidecahedron structure. It was shown that a change in the fluid conductivity results in only a slight increase in the effective thermal conductivity. For an aluminum foam ($k_s = 218 \text{ W m}^{-1} \text{ K}^{-1}$) with 95% porosity in vacuum, the three-dimensional model predicted k_{eff} to be $3.82 \text{ W m}^{-1} \text{ K}^{-1}$. Using air as the saturated fluid increases the thermal conductivity to $3.85 \text{ W m}^{-1} \text{ K}^{-1}$, while the use of water increases the thermal conductivity to $4.69 \text{ W m}^{-1} \text{ K}^{-1}$. To obtain the equation for the effective thermal conductivity of open-cell metal foam, Bhattacharya *et al.* [26] presented comprehensive analytical and experimental investigations on the determination of the effective thermal conductivity for high-porosity metal foam. A series of equations were developed to represent the thermal conductivities in different layers. Kim *et al.* [27] investigated steady forced convection flow through an aluminum foam in an asymmetrically heated channel and noted that the inertial coefficient of the metal foam is a function of friction factor for steady flow through the porous channel. Boomsma *et al.* [28] numerically studied the steady flow through open-cell metal foams using a new approach based on a fundamental periodic unit of eight cells. Their results of pressure drop for the flow through the cellular unit were compared on a length-normalized basis against experimental data. They postulated that the discrepancy between the two sets of data may be caused by the lack of pressure drop-increasing wall effects in their simulations.

Due to the enhanced heat transfer in metal foam, some applications of using metal foams as heat sinks and heat exchangers were investigated. Lu [29] numerically studied the heat transfer efficiency of metal honeycombs for thermal management applications in high-power electronics. His results demonstrated that heat transfer performance would be further improved if a honeycomb heat sink were to be designed for turbulent flow. Bhattacharya and Mahajan [30] designed finned metal foam heat sinks with 5 pores per linear inch (PPI) and 20 PPI pore densities for electronics cooling in forced convection. Their test data indicated that the 5 PPI sample resulted in higher heat transfer coefficient compared to the 20 PPI sample for a given pressure drop or fan power. Boomsma and Poulikakos [31] investigated the characteristics of water flow through aluminum foams with different compression and pore sizes. Their results revealed that the permeability and the form coefficient accurately described the pressure drop versus flow velocity behavior in porous media. Ko and Anand [32] investigated forced convection in a rectangular channel inserted with metal foam baffles. They reported that the friction factor decreased slightly with an increase in the Reynolds number and increased with baffle thickness and pore density. Boomsma *et al.* [33] experimentally studied the metal foam as a compact heat exchanger and compared its performance with a traditional heat exchanger. Their results showed that the heat exchangers made of compressed open-cell aluminum foam generated thermal resistances that were two to three times lower than the best commercially available heat exchangers. Hsieh *et al.* [34] performed an experimental investigation of heat transfer in aluminum foam heat sinks and studied the effects of porosity, pore density and flow velocity on the heat transfer characteristics. The phenomenon of local thermal nonequilibrium (LTNE) was also observed and the deduced temperature difference between the solid

and fluid phases clearly indicated the existence of non-local thermal equilibrium conditions within the heat sink. Leong and Jin [35,36] and Jin and Leong [37,38] reported a series of experimental and numerical investigations on the heat transfer performance of the different metal foams subjected to oscillating flow. Their results showed that high heat transfer performance of metal foam subjected to oscillating flow can be obtained with moderate pumping power. Dukhan and co-workers [39–42] experimentally and theoretically studied pressure drop and heat transfer in the standard and compressed metal foams. It was found that pressure drops for high pore density and compressed foams are significantly higher than those for low pore density and uncompressed foams. In addition, they reported a one-dimensional model by treating the foam as a fin using air as the working fluid and verified the model by direct experiments.

10.1.2

Oscillating Flow Through Porous Media

Early studies of oscillating flow behavior were conducted by Womersley [43] and Uchida [44] for an empty channel or tube. The features of pressure drop for oscillating flow are of crucial importance for designing cryocoolers or regenerators with inserted porous media. Investigations were performed on oscillating flow through a channel filled with particles and woven screens using both analytical and experimental methods [45–47]. Recently, Tanaka *et al.* [48] experimentally investigated fluid flow in wire screens and sponge metals under oscillating flow and obtained an empirical equation for the friction factor in terms of the hydraulic wire diameter-based Reynolds number. However, their results were subjected to a single flow displacement, and the effects of oscillatory frequency were not considered. Khodadadi [49] treated analytically the problem of oscillating flow through a porous medium channel bounded by two impermeable parallel plates with the assumption of negligible inertia effects. The results showed that oscillatory flow in porous media was dependent on the porous medium shape parameter and Stokes number. When a highly viscous fluid undergoes slow pulsation in a porous medium with high porosity, the phase lag vanishes and similar velocity profiles in the same phase with that of the pressure gradient wave were observed. Kim *et al.* [50] numerically studied the heat transfer between the channel wall and the fluid of a porous channel subjected to pulsating flow. In their computations, the local thermal equilibrium (LTE) model was assumed which led to a model of one energy equation. Their results showed that when the Darcy number is large, velocity profiles at low frequency were akin to quasi-steady flows in a nonporous channel, and for high frequency, only a narrow portion very close to the wall is affected.

To obtain the appropriate governing parameters for the oscillatory flow through a packed channel, Zhao and Cheng [51] experimentally investigated pressure drop characteristics in a packed column which consisted of three different sizes of woven screens subjected to a periodically reversing flow of air. They showed that the oscillatory pressure drop factor increases with the maximum fluid displacement and the oscillation frequency. The correlation equation obtained by Zhao and Cheng [51]

indicated that the friction factor of oscillating flow in woven screens is governed by the kinetic Reynolds number and the dimensionless flow amplitude. In addition, Zhao and Cheng [52] investigated experimentally the transition to turbulence of an oscillatory air flow in a pipe and obtained a correlation equation for the prediction of the onset of turbulence. Ju and Zhou [53] studied the oscillating pressure drop and phase shift characteristics for a regenerator filled with wire screens under high-frequency oscillation and concluded that the values for the average pressure drop in the oscillating flow are about two to three times higher than that in steady flow at the same Reynolds numbers. Wakeland and Keolian [54] reported the pressure losses across single screens subjected to low-frequency oscillating flow. The friction factor was found to depend on Reynolds number, but not on the oscillatory amplitude over the range of conditions measured.

The fully interconnected and reticulated structures with open cells of the metal foam lend themselves to many applications. Takahashi *et al.* [55] dealt with the characteristics of foamed metals as matrices of regenerators used in Stirling engines and derived the generalized experimental equations of flow friction and heat transfer for matrices of stacked foamed metals. Fu *et al.* [56,57] investigated the heat transfer in a channel filled with aluminum foams of different pore densities and reticulated vitreous carbon (RVC) foams subjected to oscillating flow. Leong and Jin [58,59] studied experimentally the effects of oscillatory frequency and flow displacement on heat transfer in metal foams subjected to oscillating flow. Their results revealed that the oscillating flow behavior is governed by the oscillatory frequency and flow displacement and that heat transfer in oscillating flow is significantly enhanced by employing open-cell metal foams in a plate channel. Based on the results for oscillating flow through a porous channel presented by Zhao and Cheng [51], Leong and Jin [60] investigated oscillating flow in open-cell metal foams and proposed a correlation equation for the friction factor in terms of the hydraulic ligament diameter-based kinetic Reynolds number and dimensionless flow amplitude. Furthermore, Jin and Leong [61] reported an experimental study of oscillating heat transfer through metal foam channel for the application of electronic cooling.

The above literature review shows that most studies of fluid flow and heat transfer in open-cell porous media were conducted for the conditions of steady and unidirectional flows. Investigations on oscillating flow through open-cell foams are relatively scarce. In the following sections, the discussion will focus on studies of oscillating flow through aluminum foams of various pore densities, which possess high thermal conductivity and its applications in thermal management.

10.2

Fluid Behavior of Oscillatory Flow in Open-Cell Metal Foams

The open-cell metal foams to be discussed mainly in this chapter are aluminum foams with different pore densities. The density and cell size of typical foams such as Duocel manufactured by ERG Materials and Aerospace Corporation are expressed in terms of pores per linear inch (PPI) and can be varied independently to match the

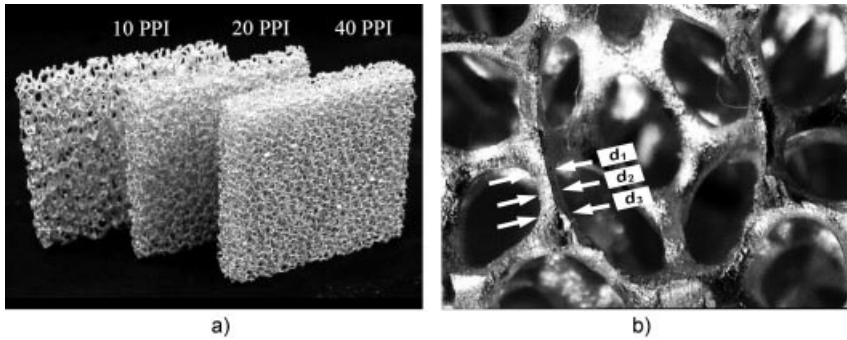


Figure 10.2 (a) Appearance of 10, 20 and 40 PPI aluminum foams and (b) typical internal structure of aluminum foam [59].

properties of the material to meet specific design requirements. Figures 10.2a and b show the typical 10, 20 and 40 PPI aluminum foams and the internal structure.

The solid metal ligament's purity of aluminum foam is typically that of the parent alloy metal with no voids and inclusions. As compared with other metal porous media, the open-cell aluminum foam is a rigid, highly porous and permeable structure with a controlled density of metal per unit volume. The matrix of cells and ligaments is completely repeatable, regular and uniform throughout the entirety of the material. Density is continuously variable from 3 to 12% and cell density can be from 5 to 60 PPI. For the materials to be discussed, the middle density of 8% and the pore size of 10, 20 and 40 PPI were used to characterize the fluid flow and heat transfer in a porous channel subjected to oscillating flow.

10.2.1

Critical Properties of Open-Cell Foams

The important parameters of open-cell foams related to the flow characteristics are porosity, inertial coefficient, permeability and ligament diameter. The physical properties of the open-cell metal materials can be determined experimentally. As shown in Figure 10.2b, the aluminum foam has a reticulated structure of open, shaped cells connected by continuous solid metal ligaments. A close-up view at a single cell of open-cell metal foam shows that the cell has the approximate shape of a 12- to 14-sided polyhedron whose pentagonal or hexagonal faces are open to one another and there is a lumping of material at joints where the ligaments meet. For the 10, 20 and 40 PPI aluminum foams used in the studies of Leong and Jin [60], the ligament diameter measurements were performed using a scanning electron microscope due to the completely repeatable structure. The diameters of ten ligaments inside the metal foam were chosen randomly were measured. For every selected ligament, the diameters at three different locations were measured as illustrated in Figure 10.2b. The average value d_l is defined as the ligament diameter and used in the calculations.

Porosity is commonly defined as the total void volume divided by the total volume occupied by the solid matrix and void volume. Due to the fully interconnected and

open-cell pore structure, there is no dead end (connected only to one other pore) or isolated pores (not connected to any other pore) inside the metal foam. Therefore, the porosity ε of an open-cell metal foam can be easily obtained by measuring the total volume of the metal foam from its external dimensions and the volume of the solid fractions according to the equation

$$\varepsilon = \frac{V_t - V_s}{V_t} \quad (10.4)$$

where V_t and V_s are the total volume and the volume of solid fraction of porous material respectively.

The term *inertial coefficient* describes the effects of the local aspects of the pore space morphology on momentum transport in the porous media. The permeability is a measure of the flow conductance of the porous matrix. The permeability K and inertial coefficient F of porous media can be determined by the modified Darcy equation proposed by Hunt and Tien [62] with the measured pressure drop and flow velocity data under the steady flow condition as

$$-\frac{dP}{dL} \frac{1}{\mu u} = \frac{1}{K} + \rho_f \frac{F}{\sqrt{K}} \frac{u}{\mu} \quad (10.5)$$

By plotting the quantity

$$\left(-\frac{1}{\mu u} \right) \left(\frac{dP}{dL} \right)$$

against $\rho_f(u/\mu)$ for a range of flow rates, the permeability is obtained as the intercept and the inertial coefficient is determined from the slope. The quadratic curve fitting method is applied to obtain the values of inertial coefficient and permeability by defining

$$A = \frac{\mu}{K}; \quad B = \rho_f \frac{F}{\sqrt{K}} \quad (10.6)$$

where A and B are constants to be determined. Consequently, Eq. (10.5) can be expressed as

$$\frac{\Delta P}{L} = Au + Bu^2 \quad (10.7)$$

where ΔP is the pressure drop and L is the length of the metal foam. Figure 10.3 presents the data of pressure drop per unit length versus velocity for steady flow of air through the 10, 20 and 40 PPI aluminum foams. By fitting the second-order polynomial of Eq. (10.7) through the data points, coefficients A and B can be determined. By substituting the values of A and B into Eq. (10.6), the corresponding values for permeability K and inertial coefficient F can be obtained. The measured values of physical properties for the tested metal foams are listed in Table 10.1.

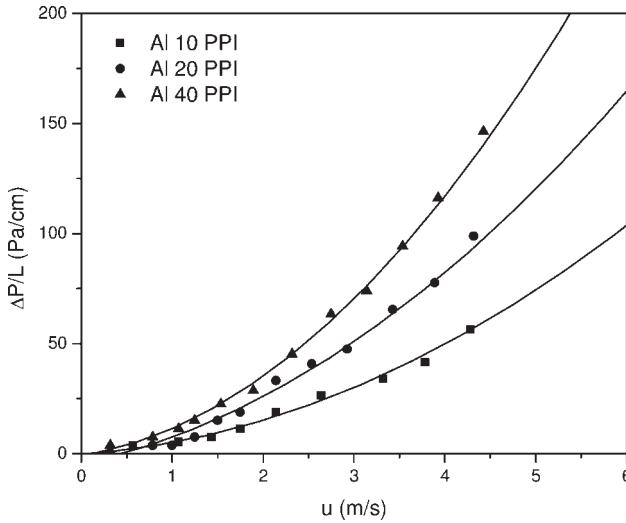


Figure 10.3 Pressure drop versus flow velocity in aluminum foams [60].

Table 10.1 Physical properties of aluminum foams [60].

Physical property	Al 10 PPI	Al 20 PPI	Al 40 PPI
Ligament diameter, d_l (μm)	427.2	221.3	112.6
Porosity, ε	0.91	0.90	0.90
Density, vol. %	8–10	8–10	8–10
Inertial coefficient, F	0.008	0.011	0.015
Permeability, K (10^{-8} m^2)	4.2	3.1	2.9

10.2.2

Analysis of Similarity Parameters

The consideration of the similarity parameters is based on the study of fully developed reciprocating flow in a circular pipe presented by Zhao and Cheng [63]. Their analysis is represented briefly below for ease of reference.

Consider fully developed oscillating flow through a circular pipe. The transient friction factor $f(\omega t)$ can be expressed as

$$f(\omega t) = \frac{\mu \left(\frac{\partial u}{\partial r} \right)_{r=D/2}}{\frac{1}{2} \rho_f u_{\max}^2} \quad (10.8)$$

where ω is the angular frequency of the imposed pressure gradient and D and r are the diameter of the pipe and the radial coordinate, respectively. Thus, the average friction factor f_{osc} in a complete oscillatory cycle is given by

$$f_{\text{osc}} = \frac{1}{2\pi} \int_0^{2\pi} |f(\omega t)| d\omega t \quad (10.9)$$

For fully developed oscillating flow through a pipe, the mass and momentum governing equations for incompressible flow are

$$\frac{\partial u}{\partial x} = 0 \quad (10.10 \text{ a})$$

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho_f} \frac{\partial P}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right) \quad (10.10 \text{ b})$$

where u is the axial velocity and ν is the kinematic viscosity of the fluid. The pressure gradient for a sinusoidal motion flow can be expressed as

$$\frac{1}{\rho_f} \frac{\partial P}{\partial x} = A_p \cos \omega t \quad (10.11)$$

where A_p is the oscillation amplitude for the imposed pressure gradient. A modified solution which is based on the result obtained by Uchida [44] for the axial velocity profile of a fully developed oscillating flow gives

$$u = \frac{A_p D^2}{Re_\omega \nu} [(1 - A) \sin \omega t + B \cos \omega t] \quad (10.12)$$

where A and B are parameters which can be determined by the kinetic Reynolds number $Re_\omega = \omega D^2 / \nu$. Re_ω was used to characterize the fluid status of oscillating flow, which could represent the periodic characteristic of oscillating flow, i.e. dimensionless oscillatory frequency. An expression of the average friction factor for oscillating flow in a pipe obtained by Zhao and Cheng [63] is

$$f_{\text{osc}} = \frac{64 F_\omega}{\pi A_0} \quad (10.13)$$

where $A_0 = x_{\text{max}} / D$ is the dimensionless flow amplitude and x_{max} is the maximum flow displacement. The function F_ω can be expressed as

$$F_\omega = \frac{\sqrt{C_1^2 + C_2^2}}{16 \sqrt{\left(\frac{1}{2} \sqrt{Re_\omega} - 2C_1\right)^2 + 4C_2^2}} \quad (10.14)$$

where C_1 and C_2 are variables given by

$$C_1 = \frac{\text{ber}\left(\frac{1}{2} \sqrt{Re_\omega}\right) \text{bei}'\left(\frac{1}{2} \sqrt{Re_\omega}\right) - \text{bei}\left(\frac{1}{2} \sqrt{Re_\omega}\right) \text{ber}'\left(\frac{1}{2} \sqrt{Re_\omega}\right)}{\text{ber}^2\left(\frac{1}{2} \sqrt{Re_\omega}\right) + \text{bei}^2\left(\frac{1}{2} \sqrt{Re_\omega}\right)} \quad (10.15 \text{ a})$$

$$C_2 = \frac{\text{ber}\left(\frac{1}{2} \sqrt{Re_\omega}\right) \text{ber}'\left(\frac{1}{2} \sqrt{Re_\omega}\right) + \text{bei}\left(\frac{1}{2} \sqrt{Re_\omega}\right) \text{bei}'\left(\frac{1}{2} \sqrt{Re_\omega}\right)}{\text{ber}^2\left(\frac{1}{2} \sqrt{Re_\omega}\right) + \text{bei}^2\left(\frac{1}{2} \sqrt{Re_\omega}\right)} \quad (10.15 \text{ b})$$

in which ber and bei are the Kelvin functions. Equations (10.16) and (10.17) indicate that F_ω is governed only by the kinetic Reynolds number Re_ω . By considering Eq. (10.15), it can be deduced that the average friction factor of oscillating flow through a pipe with constant L and D is governed by the parameters of the kinetic Reynolds number and dimensionless flow amplitude, i.e.

$$f_{osc} = f(A_0, Re_\omega) \quad (10.16)$$

Furthermore, Zhao and Cheng [51] studied experimentally oscillating flow through a porous channel filled with wire screens under various flow displacements. A correlation equation for the friction factor in terms of the kinetic Reynolds number and the dimensionless fluid displacement amplitude was presented. Their results validated that the hydraulic wire diameter-based dimensionless fluid displacement and the kinetic Reynolds number are the similarity parameters for describing the friction factor of oscillating flow through a porous channel. Consider the solid components of the wire screens and metal foam as shown in Figure 10.1. It can be observed that the wires and the ligaments are the solid struts inside the woven screen and metal foam, respectively. The flow restriction and pressure drop in metal foam will be influenced significantly by the ligament shape and structure. To study the characteristics of oscillating flow in metal foams, it is necessary to employ the hydraulic ligament diameter as the geometrical length of the materials in the investigations. The effect of the open-cell foam on oscillating flow behavior is accounted for by defining the hydraulic ligament diameter of metal foam D_h as

$$D_h = \frac{\varepsilon d_l}{1 - \varepsilon} \quad (10.17)$$

where d_l and ε are the ligament diameter and porosity of the metal foam, respectively. The proposed similarity parameters of the hydraulic ligament diameter-based kinetic Reynolds number $Re_{\omega(D_h)}$ and the dimensionless fluid amplitude A_{D_h} are defined as

$$Re_{\omega(D_h)} = \frac{\omega D_h^2}{\nu} \quad (10.18)$$

$$A_{D_h} = \frac{x_{max}}{D_h} \quad (10.19)$$

According to Eqs. (10.17) to (10.19), the effect of the average ligament diameter is included in the calculations. With the definition of the hydraulic ligament diameter as the characteristic length, the maximum friction factor proposed by Tanaka *et al.* [48] for oscillating flow through porous channel can be modified as

$$f_{max} = \frac{\Delta P_{max} D_h}{\frac{1}{2} \rho_f L (u_{max})^2} \quad (10.20)$$

where $\Delta P_{\max}$ is the maximum pressure drop in porous channel and $u_{\max}$ is the maximum flow velocity.

10.2.3

Oscillatory Flow Through a Channel Filled with Open-Cell Foams

Based on the above analysis, an experimental study was performed by the authors [60] to examine oscillating flow through a channel filled with 10, 20 and 40 PPI open-cell aluminum foams. The experimental facility is shown in Figure 10.4.

The facility consists of three major parts: oscillating flow generator, velocity measurement section and test section. The oscillating flow generator consists of a compression cylinder, a piston and a crankshaft with adjustable stroke lengths that generates a sinusoidal oscillating flow. By adjusting the motor speed through a transducer, oscillating flows of different frequencies can be generated. Different oscillating amplitudes were obtained by varying the distance of the crank from the plate center. A hot-wire sensor was mounted at the center of the two ends packed with 40 mesh woven screen discs. The packed screen provides a uniform velocity profile. The velocity measured by this arrangement is approximately the same as the cross-section averaged velocity through the column due to the extremely thin velocity boundary layer in the porous media. The test section is a well-shaped block of open-cell aluminum foams (10, 20 and 40 PPI) with dimensions of $50 \times 50 \times 10$ mm. The two taps of the differential pressure transducer are located before and after the test section for pressure drop measurements.

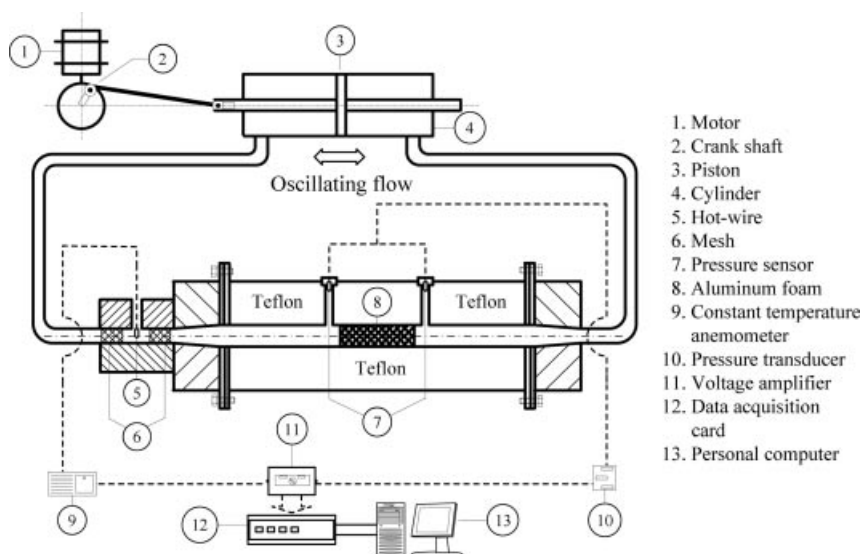


Figure 10.4 Apparatus for the measurements for oscillating flow through channel filled with aluminum foams [60].

10.2.3.1 Effects of Kinetic Reynolds Number and Dimensionless Flow Amplitude

Figures 10.5a and b present the typical variations of flow velocity and pressure drop through 10 and 20 PPI aluminum along the cycles of oscillating flow. Figure 10.5a was obtained for 10 PPI aluminum with kinetic Reynolds number $Re_{\omega(Dh)} = 24.0$,

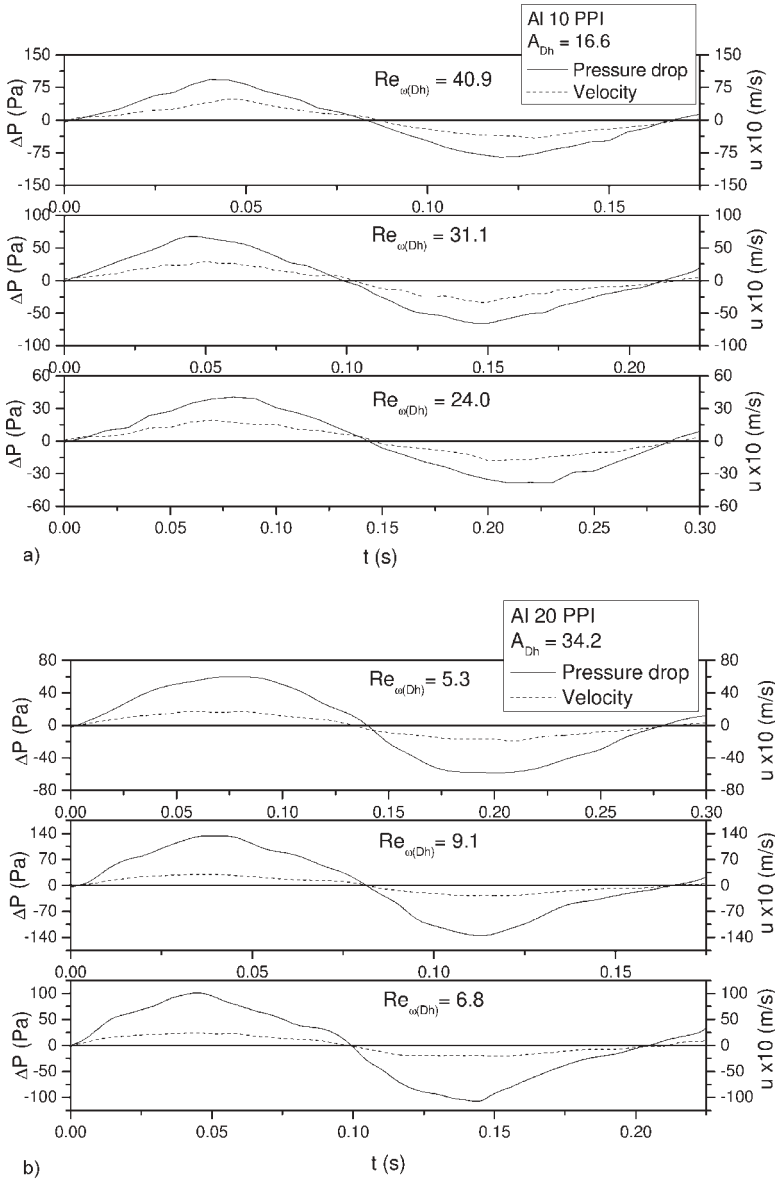


Figure 10.5 Variations of velocity and pressure drop of oscillating flow through (a) 10 PPI aluminum and (b) 20 PPI aluminum with different kinetic Reynolds number [60].

31.1 and 40.9 at the maximum flow displacement $A_{Dh} = 16.6$, and Figure 10.5b was obtained for 20 PPI aluminum with kinetic Reynolds number $Re_{o(Dh)} = 5.3, 6.8$ and 9.1 at the maximum flow displacement $A_{Dh} = 34.2$. It can be seen that the profiles of flow velocity increase with the increase of kinetic Reynolds number and vary almost sinusoidally due to the reversing flow direction. High-pressure drop corresponds to high maximum flow velocity. It is noted that the measured velocities will always be positive even though the velocity direction is reversed at every other half cycle. This is

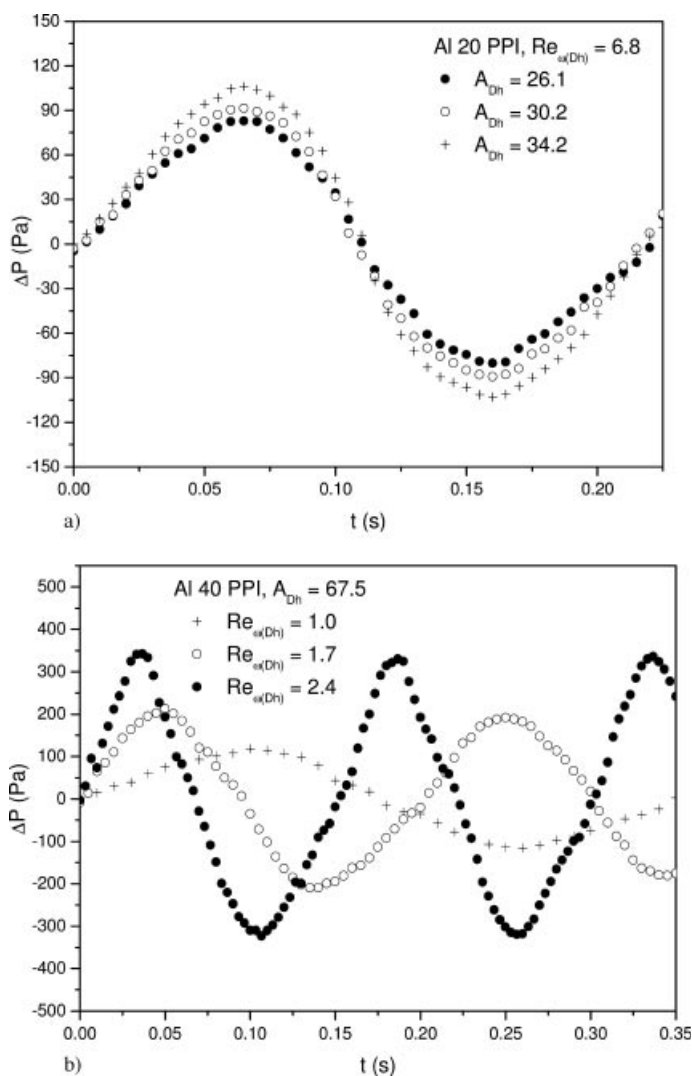


Figure 10.6 Effects of (a) maximum flow displacement and (b) kinetic Reynolds number on pressure drop in aluminum foams [60].

because of the fact that the single hot-wire sensor cannot distinguish the flow direction. To reflect a correct velocity direction, the measured values of velocity were processed by reversing its sign on every other half cycle.

To evaluate the effects of flow displacement and oscillatory frequency on the pressure drop of oscillating flow in metal foam, the pressure drop in 20 and 40 PPI aluminum foams for different cases are plotted in Figure 10.6. Figure 10.6a shows the typical temporal variations of the pressure drop across the channel filled with 20 PPI aluminum for various dimensionless flow amplitudes at a fixed kinetic Reynolds number $Re_{o(Dh)} = 6.8$. It can be seen that the pressure drop differences are only about 8–15 Pa for various flow displacements. It can also be seen that the pressure drop increases slightly with the increase of the dimensionless flow amplitude within the tested range at a fixed value of the kinetic Reynolds number. The effects of different kinetic Reynolds numbers on the variations of pressure drop across the 40 PPI aluminum foam are illustrated in Figure 10.6b for a complete cycle at $A_{Dh} = 67.5$. A difference in pressure drop of about 130 Pa is observed between the kinetic Reynolds numbers of 2.4 and 1.7. It shows that the pressure drop for high oscillatory frequency is much higher than that for low oscillatory frequency at a fixed flow displacement. These two figures indicate that the pressure drop always depends on the kinetic Reynolds number and dimensionless flow amplitude for oscillating flow through a porous channel with constant properties.

To examine the pressure drop in different materials, the variations of the maximum pressure drop in aluminum foams of 10, 20 and 40 PPI are plotted in Figure 10.7 for a given maximum flow displacement, i.e. the dimensionless flow oscillation amplitude $A_{Dh} = 14.6, 30.2$ and 59.5 for 10, 20 and 40 PPI aluminum, respectively. The oscillatory frequency was set to 3.9 Hz, i.e. the kinetic Reynolds

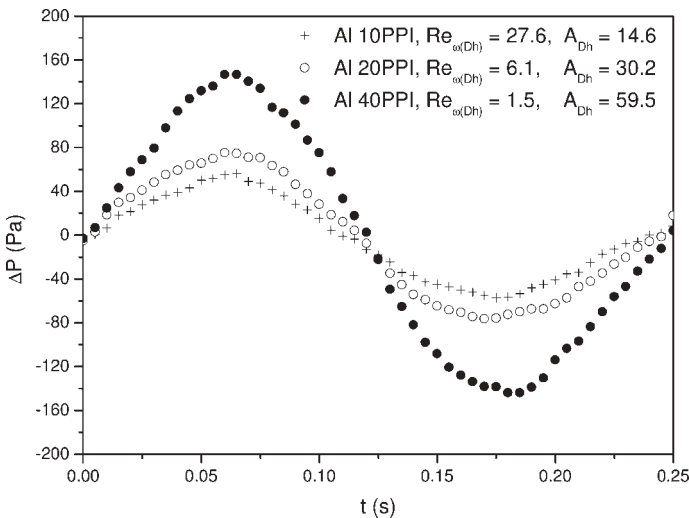


Figure 10.7 Effect of pore density on pressure drop for oscillating flow through 10, 20 and 40 PPI aluminum foams [60].

number $Re_{\omega(Dh)} = 27.6, 6.1$ and 1.5 for 10, 20 and 40 PPI aluminum, respectively. It is observed that the amplitudes of pressure drop increase markedly with the increase of the foam pore density at the same oscillation frequency. This indicates that the flow resistance in open-cell metal foam increases with the pore density.

To explain the physical meaning behind the phenomena of high pore density corresponding to high pressure drop, specific surface areas for the tested aluminum foams were examined. Lage [10] reported that the increase of flow resistance in porous materials directly relates to the effective surface length, which relates an increase in drag to the increase in specific surface area. From the metal foam specifications provided by the manufacturer [64] as shown in Figure 10.8a, the specific surface areas for 10, 20 and 40 PPI aluminum foams are approximately $790, 1750$ and $2740 \text{ m}^2 \text{ m}^{-3}$, respectively. This implies that flow resistance in high pore density metal foam is larger than that in low pore density metal foam with the same flow conditions, which is in agreement with the experimental data. Furthermore, based on Eq. (10.2) which provides the global balance of forces acting on a fully saturated permeable volume under the incompressible fluid condition, the physically meaningful ratio between the form drag and the viscous drag can be expressed as [10]

$$\frac{D_C}{D_\mu} = \frac{\rho c K}{\mu} u \quad (10.21)$$

where D_C is the form drag and D_μ is the viscous drag. Ratios of form drag to viscous drag for 10, 20 and 40 PPI aluminum foams are plotted against the flow velocity in Figure 10.8b. It can be seen that the ratio for aluminum foam with high pore density is higher than that with low pore density. This indicates that for constant porosity, the flow resistance in the tested metal foams increases with increasing form coefficient and decreasing permeability. As the flow velocity increases, the larger ratios for 40 PPI aluminum foam show that the effect of form drag on the flow resistance is more significant for pore density metal foam.

10.2.3.2 Friction Factor in Metal Foam

Based on the experimental data discussed above, Leong and Jin [60] examined the maximum friction factor of oscillating flow through the open-cell metal foam with the similarity parameters analyzed in the Section 10.2.2. The measured maximum pressure drop versus hydraulic ligament diameter-based Reynolds number is plotted in Figure 10.9a. The maximum Reynolds number based on the hydraulic ligament diameter is defined as

$$Re_{\max(Dh)} = \frac{u_{\max} D_h}{\nu_f} \quad (10.22)$$

where $u_{\max}$ is the average maximum velocity through the cross-section of porous channel. For oscillating flow through a porous channel, the maximum cross-sectional velocity $u_{\max}$ is related to the maximum flow displacement $x_{\max}$ by

$$u_{\max} = \frac{x_{\max} \omega}{2} \quad (10.23)$$

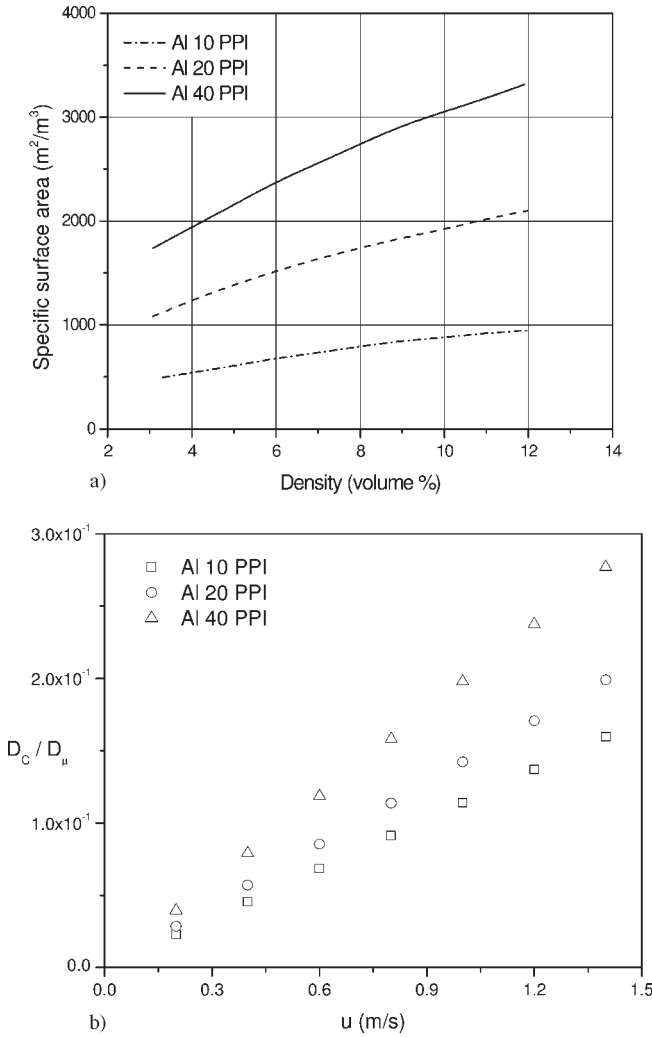


Figure 10.8 (a) Specific surface areas of 10, 20 and 40 PPI aluminum foams [64]; (b) ratio of form drag to viscous drag in 10, 20 and 40 PPI aluminum foams.

Considering Eqs. (10.18), (10.19) and (10.23), the Reynolds number in Eq. (10.22) can be expressed in terms of A_{Dh} and $Re_{\omega(Dh)}$ as

$$Re_{\max(Dh)} = \frac{A_{Dh} Re_{\omega(Dh)}}{2} \quad (10.24)$$

Figure 10.9a illustrates the kinetic Reynolds numbers $Re_{\omega(Dh)}$ versus the computed data of maximum friction factor $f_{\max}$ times the dimensionless flow displacement amplitude A_{Dh} . The data ranges of the hydraulic ligament diameter-based kinetic

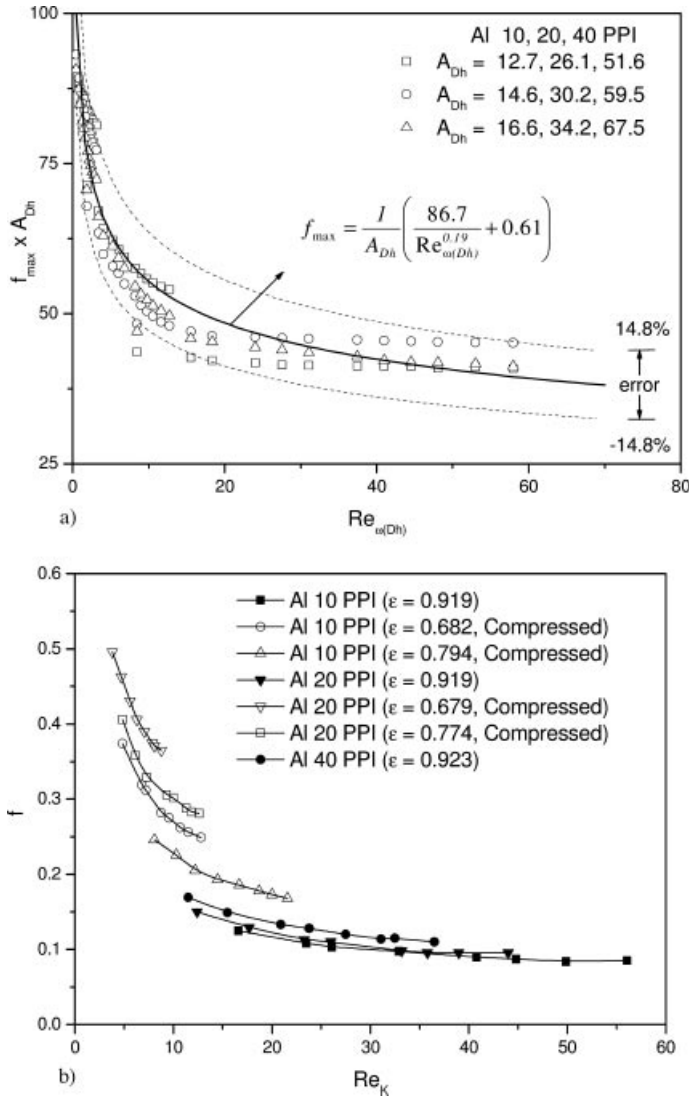


Figure 10.9 (a) Maximum friction factor for oscillating flow through 10, 20 and 40 PPI aluminum foams [60]; (b) friction factor for steady flow through various metal foams [39].

Reynolds number and dimensionless flow amplitude are $0.46 < Re_{\omega(Dh)} < 57.9$ and $12.7 < A_{Dh} < 67.5$, respectively. The following correlation for the maximum friction factor for oscillating flow in open-cell aluminum foam is obtained:

$$f_{\max} = \frac{1}{A_{Dh}} \left(\frac{86.7}{Re_{\omega(Dh)}^{0.19}} + 0.61 \right) \quad (10.25)$$

Equation (10.25) is derived from a least-squares fitting method with an error of $\pm 14.8\%$. The error range of the empirical equation plotted in Figure 10.9a shows that the friction factor of oscillating flow in metal foam is fitted well by Eq. (10.25). The correlation equation indicates that oscillating flow behavior in an open-cell metal foam is governed by the dimensionless flow displacement amplitude A_{Dh} and the kinetic Reynolds number $Re_{\omega(Dh)}$ based on the hydraulic ligament diameter of open-cell foam. The friction factors of steady air flow through various metal foams including compressed aluminum foams were investigated by Dukhan *et al.* [39]. Figure 10.9b plots their results of the friction factor versus the Reynolds number Re_K , which is defined based on the permeability K of the metal foam. The friction factor was calculated from $\Delta P \sqrt{K} / \rho L u^2$. The solid lines represent the power law fit of the experimental data. For the compressed foam, the friction factor appears to reach a constant value for Reynolds number larger than 35. The compression is seen to significantly increase the friction factor and the friction factor is higher for the 40 PPI foam as compared to that for the 10 and 20 PPI foams. This is due to the large surface area of high pore density foam, and is in agreement with the analysis presented in Figures 10.7 and 10.8.

10.3

Heat Transfer Characteristics of Oscillatory Flow in Open-Cell Foams

10.3.1

Theoretical Analysis of Forced Convection in Oscillating Flow

Fu *et al.* [57] investigated forced convection heat transfer in metal foams subjected to oscillating flow. They reported a dimensionless grouping parameter for evaluating the total heat transfer rate in metal foam channel subjected to oscillating and steady flows. In their derivation, two energy equations (i.e. local thermal nonequilibrium model) are used to account for the temperature difference between fluid and solid in the porous medium. Under the assumptions of two-dimensional, incompressible flow and uniform porosity of porous media, the energy equations of forced convection in porous medium can be expressed as [14]

$$\text{fluid phase: } \varepsilon \rho_f c_{pf} \frac{\partial T_f}{\partial t} + \rho_f c_{pf} \mathbf{u} \cdot (\nabla T_f) = \nabla \cdot (k_{fe} \nabla T_f) + h_{fs} a_{fs} (T_s - T_f) \quad (10.26a)$$

$$\text{solid phase: } (1 - \varepsilon) \rho_s c_{ps} \frac{\partial T_s}{\partial t} = \nabla \cdot (k_{se} \nabla T_s) - h_{fs} a_{fs} (T_s - T_f) \quad (10.26b)$$

where T_s , T_f , k_{se} and k_{fe} are the temperatures and effective thermal conductivities of solid and fluid phases, respectively, and h_{fs} and a_{fs} are the heat transfer coefficient and contact surface area between the solid and fluid interface. To concentrate on the analysis of forced convection heat transfer in a channel filled with porous

media, one-dimensional incompressible and fully developed flow is assumed. In addition, the properties of the porous medium are assumed to be uniform. For general porous media, the effective thermal conductivities of fluid and solid phases are approximately by

$$k_{fe} = \varepsilon k_f + k_d \quad (10.27a)$$

$$k_{se} = (1 - \varepsilon)k_s \quad (10.27b)$$

where k_d , k_f and k_s are the thermal dispersion conductivity of porous medium and the thermal conductivities of fluid and solid phases, respectively. Substituting Eq. (10.27) into Eq. (10.26), the energy governing equations can be rewritten as

$$\text{fluid phase: } \varepsilon \rho_f c_{pf} \frac{\partial T_f}{\partial t} + \rho_f c_{pf} u \frac{\partial T_f}{\partial x} = (\varepsilon k_f + k_d) \frac{\partial^2 T_f}{\partial y^2} + h_{fs} a_{fs} (T_s - T_f) \quad (10.28a)$$

$$\text{solid phase: } (1 - \varepsilon) \rho_s c_{ps} \frac{\partial T_s}{\partial t} = (1 - \varepsilon) k_s \left(\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} \right) - h_{fs} a_{fs} (T_s - T_f) \quad (10.28b)$$

In electronic cooling applications, time-averaged characteristics are of interest rather than those at a certain instant of time. Therefore, the following equations are defined as time-averaged components:

$$T_f = \bar{T}_f + \Delta T_f \quad (10.29a)$$

$$T_s = \bar{T}_s + \Delta T_s \quad (10.29b)$$

$$h_{fs} = \bar{h}_{fs} + \Delta h_{fs} \quad (10.29c)$$

$$u = \bar{u} + \Delta u \quad (10.29d)$$

where a quantity with an overbar is the time-averaged component of that quantity while a quantity with “ Δ ” is the fluctuation component of the quantity. Applying the time-averaged components of Eq. (10.29) into Eq. (10.28), the energy equations of

$$\begin{aligned} \text{fluid and solid phases are fluid phase: } & \rho_f c_{pf} \left(\bar{u} \frac{\partial \bar{T}_f}{\partial x} + \overline{\Delta u \frac{\partial (\Delta T_f)}{\partial x}} \right) \\ & = (\varepsilon k_f + k_d) \frac{\partial^2 \bar{T}_f}{\partial y^2} + \bar{h}_{fs} a_{fs} (\bar{T}_s - \bar{T}_f) + \overline{\Delta h_{fs} a_{fs} (T_s - \Delta T_f)} \end{aligned} \quad (10.30a)$$

$$\begin{aligned} \text{solid phase: } & 0 = (1 - \varepsilon) k_s \left(\frac{\partial^2 \bar{T}_s}{\partial x^2} + \frac{\partial^2 \bar{T}_s}{\partial y^2} \right) - \bar{h}_{fs} a_{fs} (\bar{T}_s - \bar{T}_f) - \overline{\Delta h_{fs} a_{fs} (T_s - \Delta T_f)} \end{aligned} \quad (10.30b)$$

Substituting the following equation into Eq. (10.30a):

$$[\bar{h}_{fs}a_{fs}(\bar{T}_s - \bar{T}_f) + \overline{\Delta h_{fs}a_{fs}(T_s - \Delta T_f)}] = (1 - \varepsilon)k_s \left(\frac{\partial^2 \bar{T}_s}{\partial x^2} + \frac{\partial^2 \bar{T}_s}{\partial y^2} \right) \quad (10.31)$$

the fluid phase energy equation can be re-written as

$$\rho_f c_{pf} \left(\bar{u} \frac{\partial \bar{T}_f}{\partial x} + \overline{\Delta u \frac{\partial(\Delta T_f)}{\partial x}} \right) = (\varepsilon k_f + k_d) \frac{\partial^2 \bar{T}_f}{\partial y^2} + (1 - \varepsilon)k_s \left(\frac{\partial^2 \bar{T}_s}{\partial x^2} + \frac{\partial^2 \bar{T}_s}{\partial y^2} \right) \quad (10.32)$$

The term

$$\overline{\Delta u \frac{\partial(\Delta T_f)}{\partial x}}$$

can be neglected because it is small compared to the average convection term $\bar{u}(\partial \bar{T}_f / \partial x)$. Equation (10.32) can now be rewritten as

$$\rho_f c_{pf} \bar{u} \frac{\partial \bar{T}_f}{\partial x} = (\varepsilon k_f + k_d) \frac{\partial^2 \bar{T}_f}{\partial y^2} + (1 - \varepsilon)k_s \left(\frac{\partial^2 \bar{T}_s}{\partial x^2} + \frac{\partial^2 \bar{T}_s}{\partial y^2} \right) \quad (10.33)$$

Based on the condition of constant heat flux at the bottom wall along the x axial direction, Eq. (10.33) can be reduced to

$$\rho_f c_{pf} \bar{u} \frac{\partial \bar{T}_f}{\partial x} = (\varepsilon k_f + k_d) \frac{\partial^2 \bar{T}_f}{\partial y^2} + (1 - \varepsilon)k_s \frac{\partial^2 \bar{T}_s}{\partial y^2} \quad (10.34)$$

For the scale analyses of the heat transfer in a porous channel, the overbar in Eq. (10.34) is dropped for simplicity. The scale analysis can be expressed as

$$\rho_f c_{pf} u \frac{\Delta T}{x} \sim (\varepsilon k_f + k_d) \frac{\Delta T}{\delta_t^2} + (1 - \varepsilon)k_s \frac{\Delta T}{\delta_t^2} \quad (10.35)$$

where ΔT is the temperature difference of the hot wall surface and the bulk temperature of the fluid and δ_t is the thickness of the thermal boundary layer. It is noted that the temperature scales for solid and fluid phases are assumed to be the same. Equation (10.35) can be rearranged as

$$\frac{\delta_t^2}{x^2} \sim \frac{[\varepsilon k_f + k_d + (1 - \varepsilon)k_s]}{\rho_f c_{pf} u x} \quad (10.36)$$

Definitions of the effective thermal conductivity k_{eff} , effective thermal diffusivity α^* of porous media and the effective local Peclet number Pe_x^* are given as

$$k_{\text{eff}} = \varepsilon k_f + k_d + (1 - \varepsilon)k_s \quad (10.37a)$$

$$\alpha^* = \frac{k_{\text{eff}}}{\rho_f c_{pf}} \quad (10.37b)$$

$$Pe_x^* = \frac{ux}{\alpha^*} \quad (10.37c)$$

Note that Pe_x^* is a function of x . Substituting Eqs. (10.37a)–(10.37c) into Eq. (10.36) gives

$$\frac{\delta_t}{x} \sim \left(\frac{ux}{\alpha^*} \right)^{-1/2} = Pe_x^{*-1/2} \quad (10.38)$$

The local Nusselt number Nu_x can be expressed as

$$Nu_x = h_x \frac{D_e}{k_f} \sim \frac{k_{\text{eff}}}{\delta_t} \frac{D_e}{k_f} = \left(\frac{k_{\text{eff}}}{k_f} \right) \left(\frac{D_e}{x} \right) (Pe_x^*)^{1/2} \quad (10.39)$$

where D_e is the hydraulic diameter of channel. The length-averaged Nusselt number is given by [65]

$$Nu_{\text{avg}} = \frac{1}{L} \int_0^L Nu_x dx = \frac{1}{L} \int_0^L \left(\frac{k_{\text{eff}}}{k_f} \right) \left(\frac{D_e}{x} \right) \left(\frac{ux}{\alpha^*} \right)^{1/2} dx \quad (10.40)$$

Performing the integration of the local Nusselt number over the entire length of the porous channel along the flow direction, the scale analysis of the length-averaged Nusselt number can be obtained as

$$Nu_{\text{avg}} \sim \left(\frac{k_{\text{eff}}}{k_f} \right) \left(\frac{D_e}{L} \right)^{1/2} (Pe^*)^{1/2} \quad (10.41)$$

where $Pe^* = uD_e/\alpha^*$ is the Peclet number based on the hydraulic diameter of the channel. Equation (10.41) implies that grouping parameter

$$\left(\frac{k_{\text{eff}}}{k_f} \right) \left(\frac{D_e}{L} \right)^{1/2} (Pe^*)^{1/2}$$

is a function of the length averaged Nusselt number for forced convection heat transfer in porous media.

10.3.2

Oscillatory Heat Transfer in Open-Cell Metal Foams

To perform the experiments for studying heat transfer in open-cell metal foams subjected to oscillating flow, the test section in the setup illustrated in Figure 10.4 was modified. A film heater was firmly mounted on the bottom of the channel to supply a constant heat flux. A 1 mm thick copper plate with eight narrow slots was attached on the surface of film heater to allow thermocouples to be positioned along the test section. The dimensionless locations of these thermocouples in terms of x/D_e (where $D_e = 5H/3$ is the hydraulic diameter of the channel) are 0, 0.4284, 0.8568, 1.2858, 1.7142, 2.1456, 2.5716 and 3. The other two thermocouples were placed at the inlet and outlet to measure the bulk temperatures. Two pairs of the cooler were attached at the two ends of the test section to remove the heat carried out by fluid flow. Details of the heat transfer experiments can be found in Ref. [58].

The heat transfer experimental data of both porous and empty channels subjected to oscillating flow conditions are shown in Figure 10.10. Figure 10.10a presents the cycle-averaged local surface temperature distribution on the substrate surface along the axial direction in oscillating flow with oscillatory frequency from 3.1 to 3.8 Hz for the empty and porous channels with different power inputs. For both the channels, there are two thermal entrance regions in the test section due to the reversing flow direction. The surface temperatures located at the two entrances are lower than that at the center of the test section. The local surface temperature distribution curves are convex with the maximum at the center of the test section. It is obvious that for different input powers, the surface temperature profile in the empty channel is much higher than that in channel filled with metal foam. The advantages of large surface area-to-volume ratio of the porous foam and intense fluid within the metal foam resulted in a much lower surface temperature distribution in a porous channel subjected to oscillating flow. Figure 10.10b shows the cycle-averaged local Nusselt number ($Nu_x = h_x D_e / k_f$) in both empty and porous channels along the dimensionless axial distance. It can be seen that the cycle-averaged local Nusselt number decreases as the dimensionless location x/D_e approaches the center of the test section. The Nusselt number distribution curves are concave with the minimum around the center of the test section as the symmetric point. It is obvious that the cycle-averaged Nusselt number for oscillating flow in porous channel is much higher than that in an empty channel. For the 40 PPI aluminum foam channel, the average Nusselt number derived from the cycle-average local Nusselt numbers of Figure 10.10b is about 3 times larger than that in empty channel. It is noted that the difference of cycle-averaged local Nusselt numbers between the two ends of the test section and center of the porous channel is larger than that in empty channel. This indicates that heat transfer performance can be significantly enhanced at the thermal entrance region in oscillating flow through a channel filled with metal foam.

One direct reason for the difference of thermal performance between oscillating flow through porous and empty channels is the difference of effective thermal conductivity between the porous and empty channels. Calmidi and Mahajan [24] obtained a correlation for the effective thermal conductivity k_{eff} for aluminum

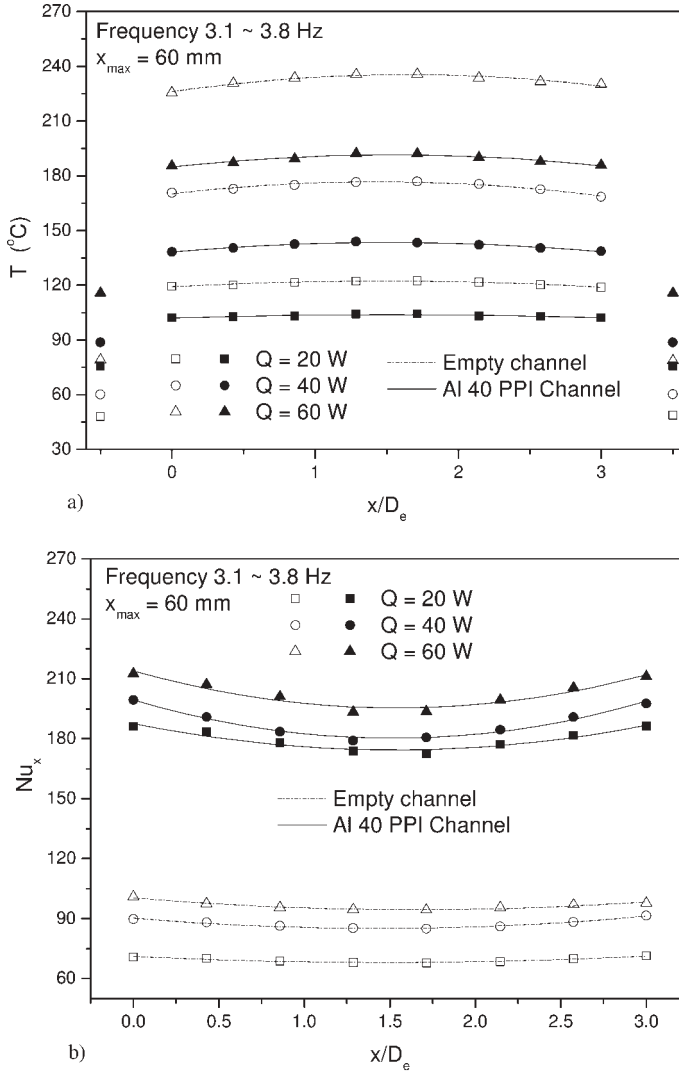


Figure 10.10 Comparison of heat transfer in oscillating flow through porous and empty channel: (a) cycle-averaged surface temperature distribution; (b) cycle-averaged local Nusselt number distribution [58].

foams, which are the same materials studied by Leong and Jin [58]. Their equation is

$$k_{\text{eff}} = \varepsilon k_f + 0.181(1 - \varepsilon)^{0.762} k_s \quad (10.42)$$

Using Eq. (10.42), the variation of effective thermal conductivity of oscillating flow through the channel filled with 40 PPI aluminum foam is shown in Figure 10.11. It

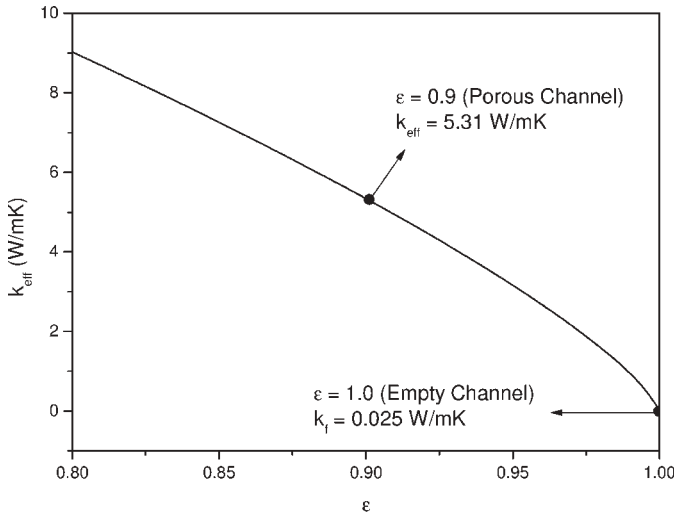


Figure 10.11 Variation of the effective thermal conductivities with the porosities of the channel.

should be noted that for $\epsilon = 1$, i.e. empty channel, the effective thermal conductivity is equal to the fluid thermal conductivity. It can be seen that the effective thermal conductivity decreases with an increase of the porosity of the metal foam. Comparing the tested porous channel ($\epsilon = 0.9$) and empty channel ($\epsilon = 1$), it can be seen that the effective thermal conductivity in the metal foam is much higher than that in an empty channel. The large difference in the effective thermal conductivity results in high heat transfer rate achieved by oscillating flow through a metal foam as compared to that through an empty channel.

10.3.3

Effects of Oscillation Frequency and Flow Amplitude

The discussion of the fluid behavior in open-cell metal foam presented in Section 10.2 shows that oscillatory frequency and flow amplitude are the critical factors for oscillating flow through a porous channel. To reveal the effects of oscillatory frequency and maximum flow displacement on the heat transfer, the dimensionless flow amplitude $A_0 = x_{\text{max}}/D_e$ and kinetic Reynolds number $Re_{\omega} = \omega D_e^2/\nu$ were employed to study the heat transfer characteristics of oscillating flow through metal foam channel. To focus the discussion on the effects of flow parameters on heat transfer in metal foams, the 40 PPI aluminum foam was tested for various flow conditions. The discussion on oscillating flow through different aluminum foams is found in Section 10.1.2.

The effect of kinetic Reynolds number on the cycle-averaged local surface temperature of 40 PPI aluminum foam for amplitude of flow displacement $A_0 = 3.6$ is presented in Figure 10.12a. It can be observed that the cycle-averaged local surface temperature profile decreases with the increase of the kinetic Reynolds number for different flow displacements. This implies that high oscillatory frequency corresponds

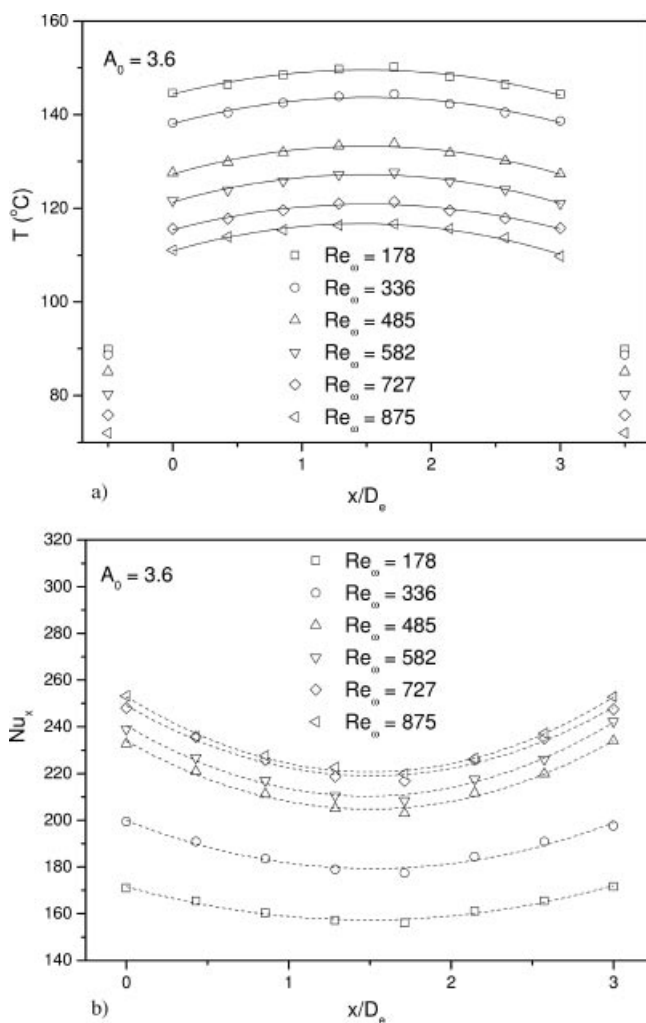


Figure 10.12 Effects of kinetic Reynolds number on (a) cycle-averaged local surface temperature and (b) cycle-averaged Nusselt number distributions.

to low surface temperature in the tested range. As shown in the figure, a temperature difference of approximately 30–40 $^{\circ}\text{C}$ can be achieved between the maximum and minimum kinetic Reynolds numbers for $A_0 = 3.6$. Figure 10.12b presents the distributions of the calculated local Nusselt numbers for oscillating flow corresponding to various kinetic Reynolds numbers. It shows that the cycle-averaged local Nusselt number increases with the increase of kinetic Reynolds number, i.e. oscillatory frequency. Physically, a higher oscillatory frequency means a shorter cycle time for the oscillating flow to reverse its direction. It implies that for a certain cooling period, high frequency results in cooler fluid entering the porous channel alternately from the two

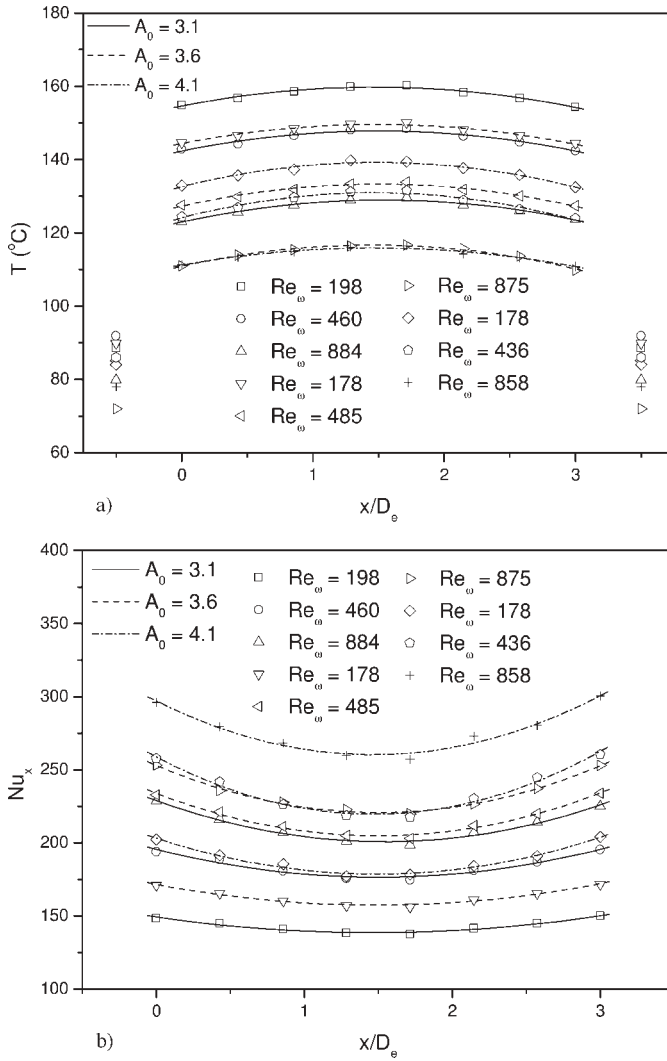


Figure 10.13 Effects of dimensionless flow amplitude on (a) the cycle-averaged local surface temperature and (b) the cycle-averaged Nusselt number distributions with different kinetic Reynolds numbers.

inlets and enhanced heat transfer performance. It can also be seen that for varying oscillatory frequency, the distribution curves of the cycle-averaged local Nusselt number are concave about the center of the test section as the symmetric point.

The effect of dimensionless amplitude of flow displacement A_0 on heat transfer of oscillating flow in a porous channel with different kinetic Reynolds numbers is also presented in Figure 10.13. It can be seen from Figure 10.13a that the temperature profile decreases with an increase in the dimensionless amplitude of flow

displacement for various kinetic Reynolds numbers. For different flow amplitudes and kinetic Reynolds numbers, the cycle-averaged local surface temperature distributions are similar to the results in Figure 10.12a. The effect of dimensionless flow amplitude A_0 on the distribution of cycle-averaged Nusselt number at different Reynolds numbers is shown in Figure 10.13b. It is clear that the profile of cycle-averaged local Nusselt number for large A_0 is higher than that for small A_0 . A closer observation shows that for large displacements, the variation of the Nusselt number along the axial direction is larger than that for small displacements. This implies that the thermal entrance region for oscillating flow with large amplitude of displacement is longer than that for oscillating flow with small amplitude of displacement. Within the tested ranges of frequency and flow amplitude, it can be deduced that higher heat transfer rates can be obtained by larger displacement oscillating flows with high kinetic Reynolds number in a porous channel.

10.3.4

Heat Transfer Rate in Metal Foams

In order to evaluate the overall effects of dimensionless amplitude of flow displacement A_0 and kinetic Reynolds number Re_w on the total heat dissipation rate in a porous channel subjected to oscillating flow, the length-averaged Nusselt number was used. Figure 10.14a presents the length-averaged Nusselt number versus kinetic Reynolds number with different dimensionless amplitudes of flow displacement for a porous channel with $L/D_e = 3$. Generally, the length-averaged Nusselt number Nu_{avg} increases with both the dimensionless parameters A_0 and Re_w . However, it is noted that for fixed dimensionless amplitude of flow displacement A_0 , the length-averaged Nusselt number approaches a constant value for a kinetic Reynolds number Re_w of about 874. This implies that very high oscillatory frequency has very little contribution to an increase in heat transfer rate in oscillating flow through a porous channel. This suggests that oscillating flow at relatively low frequency and high amplitude of displacement has a substantial effect on the heat transfer behavior in a porous channel since the temperature fluctuation on the wall surface cannot follow the oscillatory velocity at very high frequency. Using the least squares method, the data in Figure 10.14a can be collapsed onto a fitting line as shown in Figure 10.14b. The resulting correlation equation with a error of $\pm 9.8\%$ for the length-averaged Nusselt number in terms of the dimensionless amplitude of flow displacement and kinetic Reynolds number for oscillating flow with $Re_w = 150$ to 900 and $A_0 = 3.1$ to 4.1 in a porous channel of $L/D_e = 3$ is

$$Nu_{avg} = 12.38 A_0^{0.95} Re_w^{0.31} \quad (10.43)$$

Equation (10.43) indicates that the effect of A_0 on the heat transfer behavior in oscillating flow is more dominant than that of Re_w due to the larger exponent of A_0 . It implies that higher heat transfer performance can be obtained by oscillating flow through a porous channel with relatively low frequency and high displacement.

For the transient thermal problem in porous media under oscillating flow condition, the temperature variations of the solid and fluid phases were studied

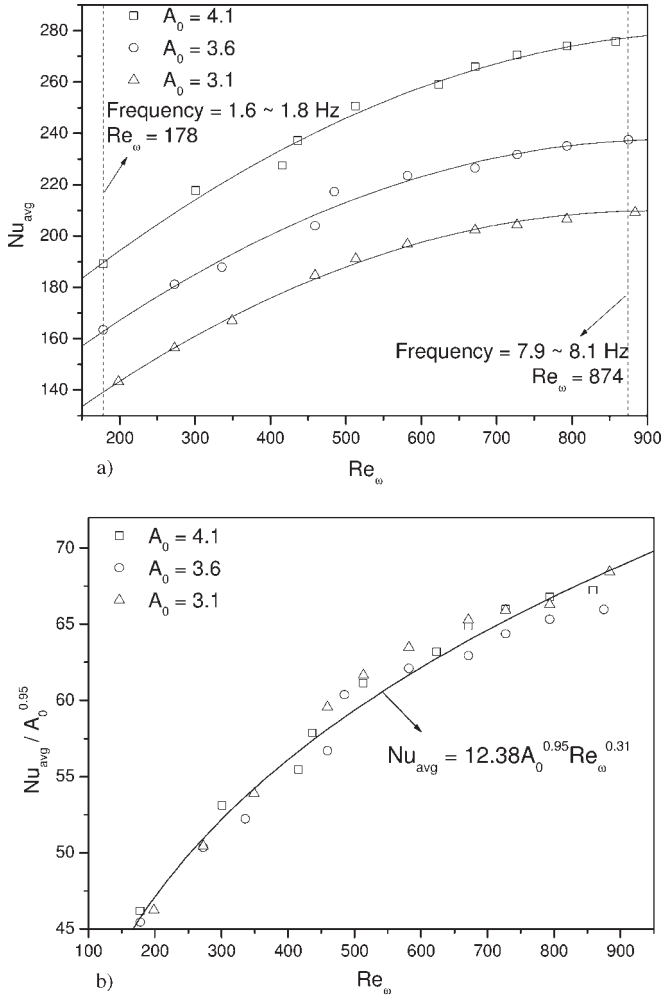


Figure 10.14 (a) Effects of A_0 and Re_ω on the length-averaged local Nusselt number; (b) correlation equation of the length-averaged local Nusselt number for oscillating flow through aluminum foam [58].

theoretically by Byun *et al.* [66]. The two temperature equations (Eqs. (10.26a,b)) can be simplified as

$$\frac{d\theta_f}{d\tau} + \cos(\tau) = N(\theta_s - \theta_f) \quad (10.44a)$$

$$M \frac{d\theta_s}{d\tau} = N(\theta_f - \theta_s) \quad (10.44b)$$

where θ is the nondimensional temperature based on the linear temperature distribution and τ is the nondimensional time. M and N are the ratios of the interstitial heat

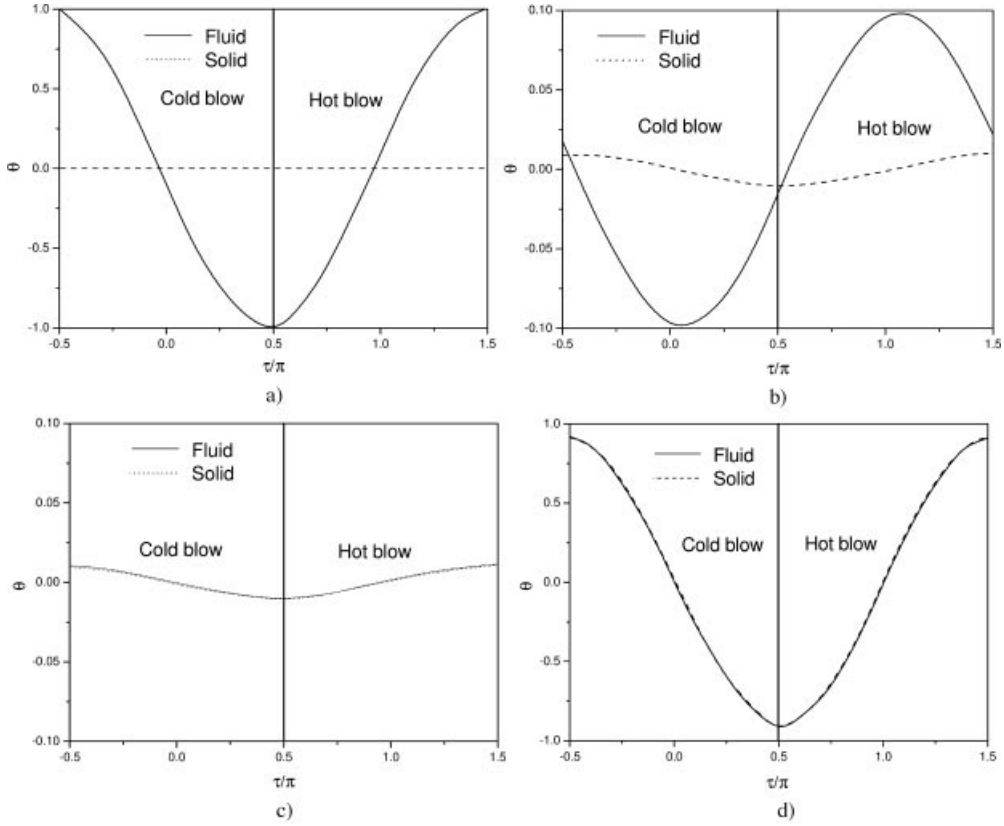


Figure 10.15 Transient temperature variations for (a) $N = 100$, $M = 0.1$; (b) $N = 100$, $M = 10$; (c) $N = 100$, $M = 1000$; (d) $N = 0.1$, $M = 10$ [66].

conductance between the phases to the fluid thermal capacity and the ratio of the thermal capacities between the solid and fluid phases, respectively, and are defined as

$$M = \frac{ha}{\varepsilon(\rho_f C_{pf})\omega} \quad (10.45a)$$

$$N = \frac{(1 - \varepsilon)(\rho_s C_{ps})}{\varepsilon(\rho_f C_{pf})} \quad (10.45b)$$

where h is the heat transfer coefficient and a is the interfacial area. These two parameters represent how fast or how large an amount of heat can be transferred from the fluid phase to the solid phase. The exact solutions were obtained for both the fluid and solid temperature variations and the results for different cases are presented in Figure 10.15. For the case of relatively large N and small M as shown in Figure 10.15a, the temperature variation of the fluid phase is very large whereas that of the solid

phase is very small. As M increases for a fixed value of N , the temperature variation of the fluid phase becomes smaller and that of solid phase becomes larger as shown in Figure 10.15b. For a further increase of M beyond the value of N , the solid temperature remains relatively constant while the fluid temperature oscillation decreases to assume a similar temperature variation as the solid phase as shown in Figure 10.15c. Meanwhile, if N decreases from the case in Figure 10.15c, the temperature oscillations increase for both the solid and fluid phases as shown in Figure 10.15d.

According to the above findings, the ratio of N to M can be used as a criterion for the validity of the local thermal equilibrium condition in this problem, which can be written as

$$\frac{N}{M} = \frac{(1 - \varepsilon)(\rho_s C_{ps})\omega}{ha} = \frac{t_p}{t_o} \leq 1 \quad (10.46)$$

with

$$t_o = \frac{1}{\omega} \quad \text{and} \quad t_p = \frac{(1 - \varepsilon)(\rho_s C_{ps})}{ha} \quad (10.47)$$

where t_o is the time scale of the variation of the flow or thermal boundary condition, and t_p is the time scale concerning the thermal inertia of the porous media. The ratio N/M can be used to verify the local thermal equilibrium condition for porous media subjected to oscillating flow. When the characteristic time of the porous media is much shorter than the time scale concerning the variation of the boundary condition, local thermal equilibrium is achieved and the temperature difference between solid and fluid phases can be neglected.

A numerical study was performed by Calmidi and Mahajan [67] to investigate forced convection in high-porosity metal foams. In their simulated domain, the bottom wall is heated under a specified temperature profile and the upper wall is insulated. The fluid is assumed to enter at a constant temperature and a zero diffusion condition is assumed for the fluid phase at the exit. The nondimensionalized transport equations are

$$\frac{dU}{dY^2} = \frac{\varepsilon}{\sqrt{Da}}(U - 1) + \frac{Re_K}{Da} F\sqrt{\varepsilon}(U^2 - 1) \quad (10.48a)$$

$$0 = \frac{1}{Bi_s} \left(\frac{d^2\theta_s}{dX^2} + \frac{d^2\theta_s}{dY^2} \right) - (\theta_s - \theta_f) \quad (10.48b)$$

$$\begin{aligned} U \frac{\partial \theta_f}{\partial X} = & \frac{\partial}{\partial X} \left(\left(\frac{Da}{Re_K Pr_{fe}} + C_D U \right) \frac{\partial \theta_f}{\partial X} \right) + \frac{\partial}{\partial Y} \left(\left(\frac{Da}{Re_K Pr_{fe}} + C_D U \right) \frac{\partial \theta_f}{\partial Y} \right) \\ & + \frac{Bi_f}{Re_K Pr_{fe}} (\theta_s - \theta_f) \end{aligned} \quad (10.48c)$$

where

$$Da = \frac{\sqrt{K}}{H}, \quad Bi_s = \frac{h_{fs} a_{fs} H^2}{k_{se}} \quad \text{and} \quad Bi_f = \frac{h_{fs} a_{fs} H^2}{k_{fe}} \quad (10.49)$$

are Darcy and Biot numbers. A fully developed velocity profile is prescribed at the inlet and the energy equations were solved using the ADI finite difference scheme.

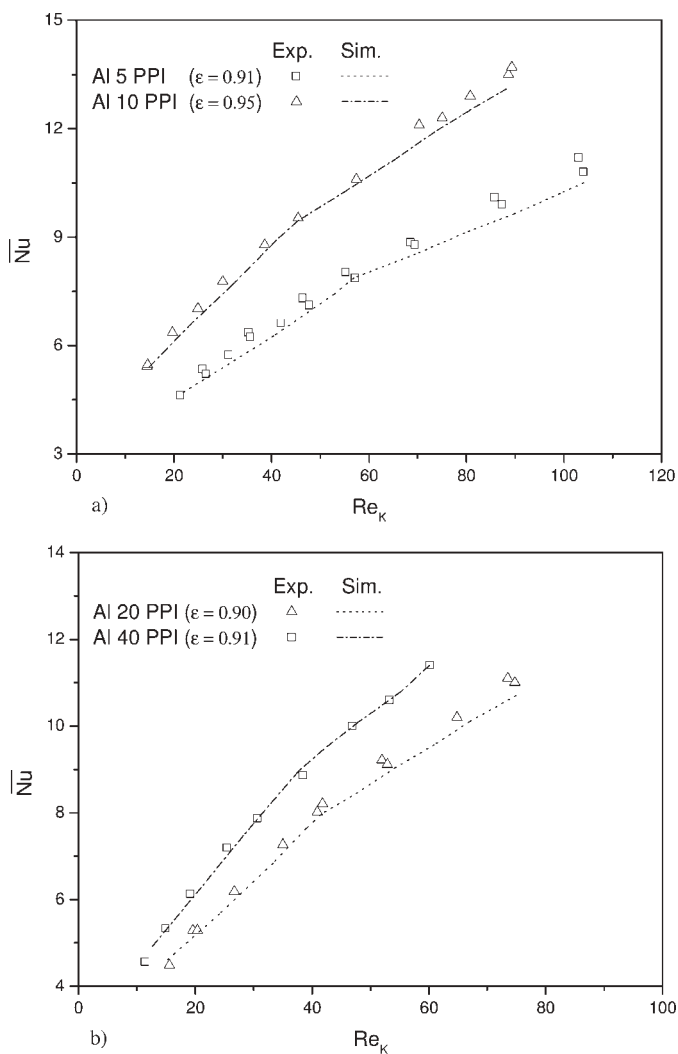


Figure 10.16 Numerical results of heat transfer of steady air flow through (a) 5 and 10 PPI aluminum foams and (b) 20 and 40 PPI aluminum foams [67].

The numerical results of average Nusselt number on the heat surface with the experimental data for 5–10 PPI aluminum foams and 20–40 PPI foams are rearranged in Figures 10.16a and b, respectively. Generally, the total heat transfer rate increases with the Reynolds number and the simulation results show a good fit with their experimental data. The largest Nusselt number was obtained for high pore density 40 PPI foam as compared to the Nusselt numbers obtained with 5, 10 and 20 PPI foams. An analysis of the results reveals a systematic deviation between the experimental and computed data for high Reynolds number. In particular, the numerical results appear to under-predict the experimental Nusselt number for $Re_K > 80$. The indication is that some other transport enhancing effect such as turbulence may have occurred in the experimental study.

10.4

Thermal Management Using Highly Conductive Metal Foams

One of the primary reasons for studying forced convection in open-cell metal foams is their possible application in electronics cooling. The fibers of the metal foam with high thermal conductivity can be thought of as a complex network of extended surfaces emanating from the substrate of the heated surface. Furthermore, when a fluid flows through the metal foam matrix, it follows tortuous paths and undergoes considerable mixing. As a result, the efficiency of heat transfer from the fibers to the fluid is enhanced. For various electronics cooling applications, heat transfer in metal foams under different flow conditions will be discussed in this section.

10.4.1

Steady and Oscillating Flows in Open-Cell Metal Foams

10.4.1.1 Thermal Performance of Open-Cell Metal Foams

For electronics cooling applications, Bhattacharya and Mahajan [30] studied the finned metal foam heat sinks proposed by Calmidi *et al.* [68] under forced convection conditions. The foams were cut into their precise geometry and inserted into the gap of the fins. Their results of the heat transfer coefficients for 20 PPI aluminum with one, two, four and six fins and the comparison with plate-finned heat sinks are shown in Figure 10.17a. For 20 PPI finned metal foams, the heat transfer coefficient h increases at a given air flow velocity u when fins were incorporated in the metal foams and the variation of h with u was found to be almost linear in the tested velocity range. Compared to the longitudinal plate-finned heat sinks, the heat transfer coefficients offered by the finned metal foams are consistently higher than those offered by the plate-finned heat sinks in the entire velocity range. Thus it can be seen that significant enhancements in heat transfer rates can be achieved by the finned metal foams. Kim *et al.* [69] compared the thermal performance between the traditional parallel-plate heat sinks and the aluminum foam blocks under steady air flow. The external dimensions of the aluminum foam heat sinks (AFHS) and parallel-plate heat sinks (PPHS) are the same. The thermal resistance of aluminum foam

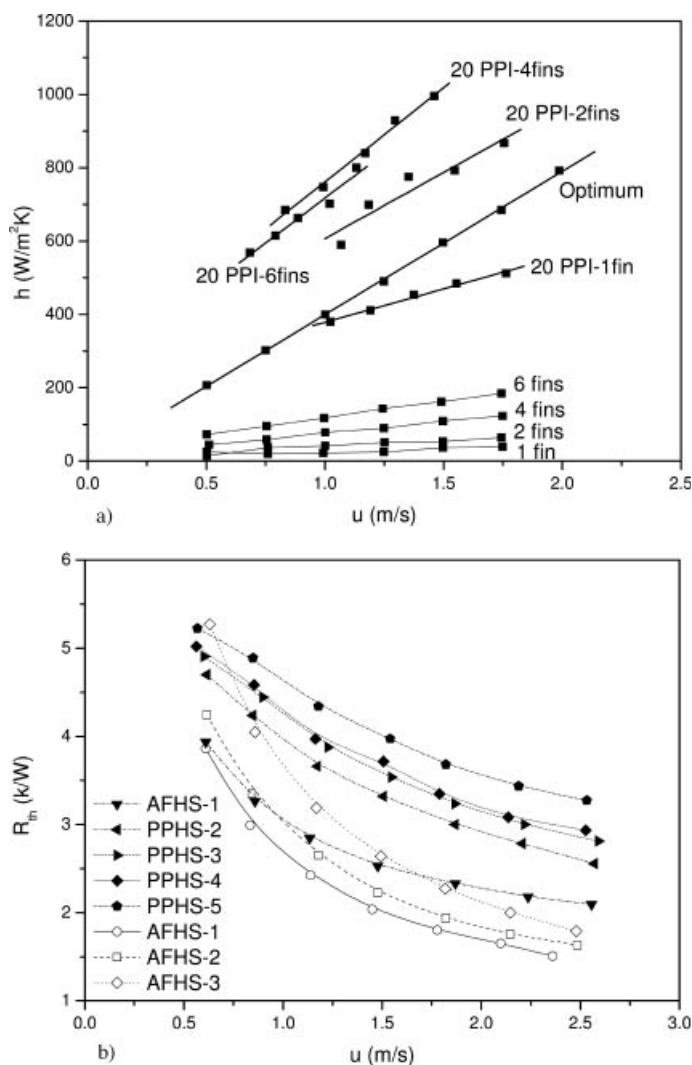


Figure 10.17 (a) Heat transfer coefficients of the finned metal foam heat sinks [30]; (b) thermal resistance of the aluminum foam heat sinks [69].

specimens AFHS-1 (10 PPI), AFHS-2 (20 PPI) and AFHS-3 (40 PPI) were measured and compared with that of conventional heat sinks of PPHS-1 to PPHS-5 (fin spacing from 6 to 14 mm). It is observed from Figure 10.17b that the thermal resistance of all the tested heat sinks decreases substantially as the inlet air velocity increases. The comparison shows that the thermal resistance of the aluminum foam heat sinks is similar to that of the parallel-plate heat sinks at low flow rates. At higher flow rates, however, the aluminum foam heat sinks show about 28% reduction in

thermal resistance compared to that in the conventional parallel-plate heat sinks. It is also noted that the mass of the aluminum heat sink is only about 25% of that of the parallel-plate heat sinks. This implies that the aluminum foam heat sinks possess advantages of better cooling performance with lower overall mass. Consequently, the aluminum foam heat sink might be very useful for compact cooling systems for electronic devices.

The metal foams were also studied as inserted materials of compact heat exchangers. Haack *et al.* [70] tested the heat transfer performance of FeCrAlY and aluminum foams with different properties using air as coolant. Their results for all tested foams are summarized in Figure 10.18a. The data of the length-averaged Nusselt numbers versus permeability based Reynolds numbers ($Re_K = u\sqrt{K}/\nu$) reveal that higher rates of heat removal were obtained by aluminum foams as compared to FeCrAlY foams. While small pore size materials can achieve higher Nusselt numbers, increasing material density was found to increase Nusselt numbers at a given rate of coolant flow. It is found that the bare metal conductivity of aluminum is approximately ten times that of FeCrAlY. However, the heat transfer performance of aluminum foam is only two to three times greater than FeCrAlY. This demonstrates that the foam structure and therefore the turbulence induced in the process fluid substantially improve heat transfer performance. Boomsma *et al.* [33] studied the heat transfer rates of compressed metal foams as compact heat exchangers subjected to steady water flow. The calculated Nusselt numbers against the water flow speed are plotted in Figure 10.18b. Their results show that all Nusselt numbers increase monotonically with increasing coolant velocity. The metal foams with the lowest Nusselt values are the two most porous foams, i.e. samples 92-02 ($\epsilon = 87.4$) and 95-02 ($\epsilon = 88.2$). The larger Nusselt numbers are obtained for samples 95-04, 95-06, 95-08, 92-03 and 92-06, which possess relatively low porosity from 60.8 to 80.5%. It is clear that the heat transfer rates of open-cell metal foams are much higher than that of the plate channel. In addition, Tadrist *et al.* [71] investigated the use of randomly stacked fibers and metallic foams in compact heat exchangers. Based on their experimental results, they suggested that the metallic foams could be used to simultaneously increase thermal efficiency without much increase in pressure drop due to the open metallic matrix.

Another cooling technique, i.e. air impingement in aluminum foams, was experimentally studied by Kim *et al.* [72]. The experiments were performed for both single and multiple air jets. The results of the heat transfer enhancement in 10, 20 and 40 PPI aluminum foams for the single- and multi-jet air impingements are presented in Figures 10.19a and b, respectively. Their results show that the aluminum foam heat sinks give between 8 and 33% higher cooling performance compared to conventional plate-fin heat sinks under single-jet impingement while the enhancement is 2–29% for multi-jet impingement. The 10 PPI aluminum foam shows a better cooling performance than the 20 and 40 PPI heat sinks under both single- and multi-jet impingements. It is noted that the 10 PPI aluminum foam has less flow resistance and results in higher mass flow rate inside the heat sink while the 40 PPI foam shows better thermal performance than the 20 PPI due to much higher heat transfer surface despite increased flow resistance.

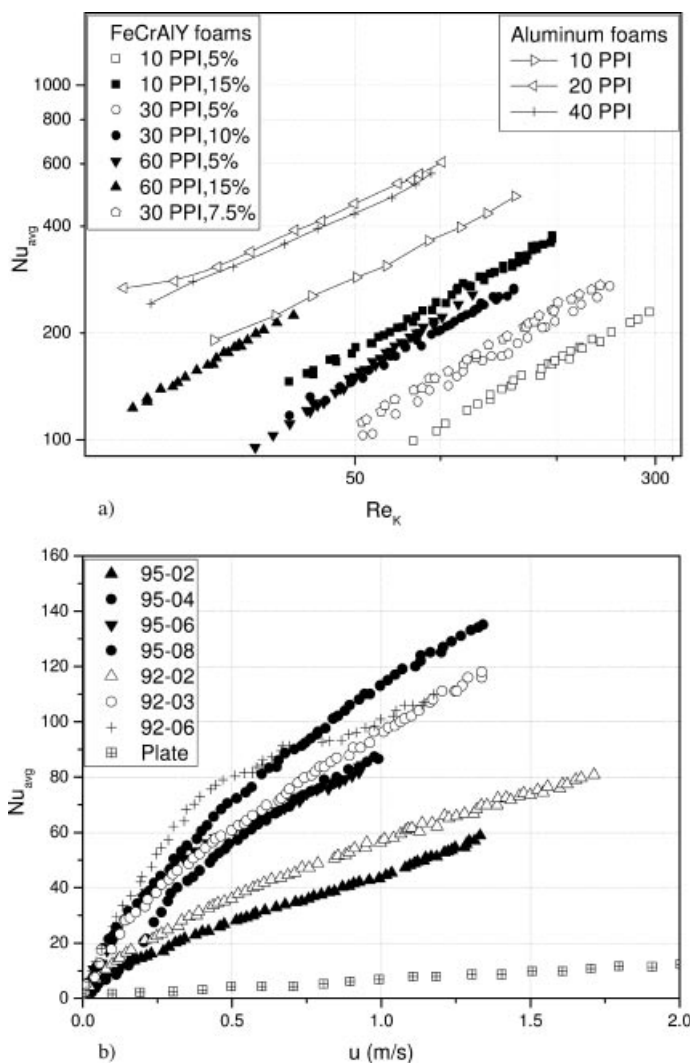


Figure 10.18 Heat transfer performance of metal foams as heat exchangers using (a) air [33] and (b) water [70] as coolants.

10.4.1.2 Comparison of Steady and Oscillating Flows

The discussions in previous sections show that open-cell metal foams can be applied in various thermal management applications. The results indicate that the thermal efficiency of highly conductive metal foams is higher than currently used designs for the same application, i.e. traditional fin heat sinks and heat exchangers with protrusions. However, most of the results were obtained under unidirectional flow conditions. To explore the advantage of using oscillating flow, it is necessary to compare the heat transfer performance between oscillating and steady flows

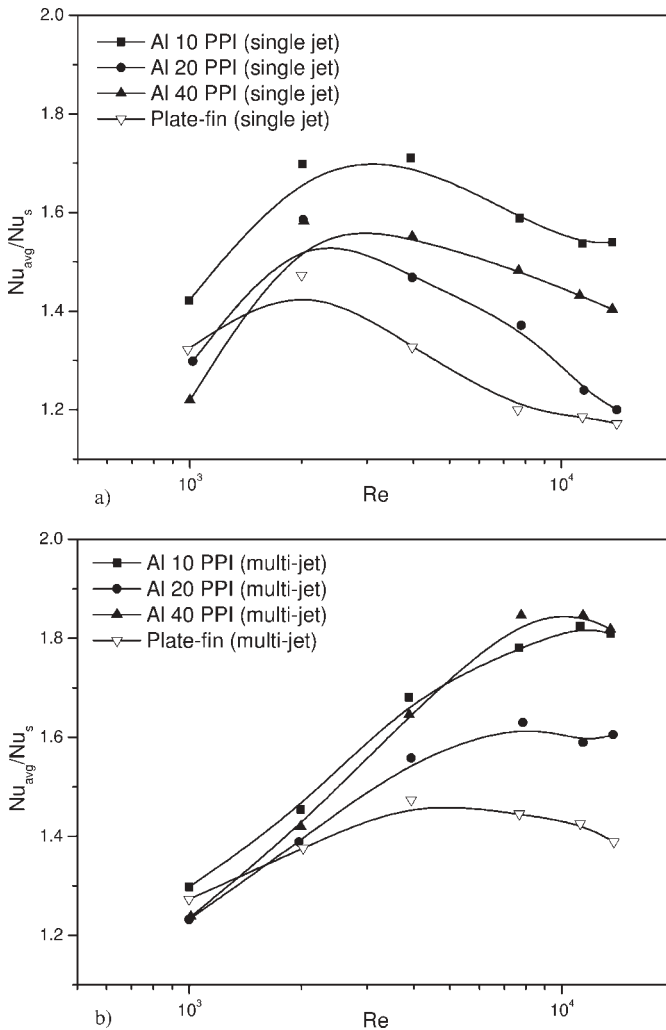


Figure 10.19 Average Nusselt number for (a) single-jet and (b) multi-jet air impingements in aluminum foams and plate-fin heat sinks [72].

through a metal foam channel by examining the temperature and Nusselt number distributions in metal foams with different pore densities. The dimensionless grouping parameter (Eq. 10.41) derived in Section 10.3.1 will be used to evaluate the thermal management performance for steady and oscillating flows through metal foams. The experimental setup shown in Figure 10.4 is also capable of performing steady flow experiments. By leaving one end of the test section open to the atmosphere, experiments of steady flow through metal foam channel can be conducted through an auto-balance compressor with the same test section configuration

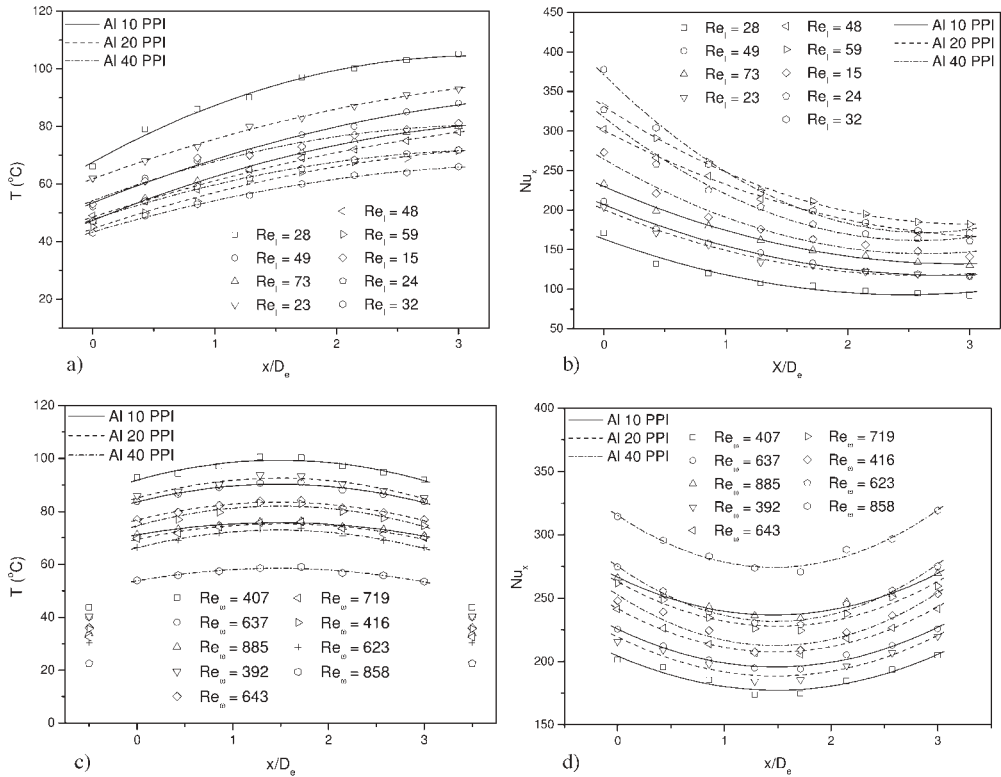


Figure 10.20 (a) Local temperature; (b) local Nusselt number distributions of steady flow through aluminum foams; (c) cycle-averaged temperature; (d) cycle-averaged local Nusselt number of oscillating flow through aluminum foams [59].

and sensors. The air flow rate was adjusted by a flow regulator and a valve installed on the mains supply.

For electronics cooling, the chip devices are susceptible to excessively high local temperatures. Therefore, the temperature distribution along the flow direction of the test section is of practical interest in design. Figures 10.20a and b present the local temperature and Nusselt number distributions, respectively, along the axial direction for steady flow through aluminum foams of 10, 20 and 40 PPI. The Reynolds number $Re_l = ud_l/\nu$ is defined based on the ligament diameter which takes into consideration the physical properties of the metal foam. From Figure 10.20a, general features of steady flow through porous channel can be observed. The local surface temperature increases with the increase of the dimensionless axial position x/D_e and the decrease of the Reynolds number. For approximately the same Reynolds number, a lower temperature distribution is obtained for higher pore density metal foam. Figure 10.20b plots the local Nusselt number distribution along the axial direction for aluminum foams under the conditions described for

Figure 10.20a. It can be seen that the local Nusselt number increases with the increase of the Reynolds number. The local Nusselt number reaches a maximum at the thermal entrance region and decreases with the increase of the axial distance for fixed Reynolds number and approaches a minimum. The variation of local Nusselt number for a lower Reynolds number along the axial direction is less significant than that for a larger Reynolds number. It can also be observed from Figure 10.19b that the profile of Nusselt number for high PPI aluminum foam is higher than that for low PPI foam under the same Reynolds number. As a comparison, Figure 10.20c presents the cycle-averaged local surface temperature of oscillating flow through 10, 20 and 40 PPI metal foam with different kinetic Reynolds numbers at $A_0 = 4.1$. It can be observed that the cycle-averaged temperature distribution in the tested foams decreases with an increase in Reynolds number. Comparing the temperature distributions in different aluminum foams at approximately the same kinetic Reynolds number, it is found that the temperature profile for high pore density foam is lower than that for low pore density foam. It is also observed that the inlet and outlet bulk temperatures (isolated points plotted in Figure 10.20c) are much lower than the temperatures in the test section due to heat removal at the coolers located at the two ends of the test section. Compared to the magnitudes of the temperature distribution of oscillating flow through the aluminum foam channel, the temperature difference between the locations of $x/D_e = 0$ and $x/D_e = 3$ for steady flow can be considered to be significant. Figure 10.20d displays the cycle-averaged local Nusselt numbers versus the dimensionless axial distance for the cases presented in Figure 10.20c. The data of the local Nusselt numbers were calculated based on the cycle-averaged local surface temperature. It can be seen that the cycle-averaged local Nusselt number in the thermal entrance region is higher than that in the location around the center of the test section. It can also be observed that the higher Nusselt number distribution was obtained by high PPI foam as compared to that of low PPI foam at the same kinetic Reynolds number.

Based on the above observations, it is shown that the temperature increases are different for steady and oscillating flows. For steady flow, the surface temperature increases along the flow direction and reaches the maximum temperature at $x/D_e = 3$. For oscillating flow, the surface temperature distribution curves are convex with the maximum value around the center of the test section. To quantify the temperature distribution uniformity for different cases, Fu *et al.* [57] defined an index I_{uni} given by

$$I_{uni} = \frac{T_{max} - T_{min}}{T_{max}} \quad (10.50)$$

where T_{max} and T_{min} are the maximum and minimum temperatures on the surface of the test section, respectively. This index represents the ratio of the maximum temperature difference to the maximum local temperature on the surface. From Eq. (10.50), a smaller value of index I_{uni} means a more uniform surface temperature distribution. When the surface temperature distribution is uniform, I_{uni} will approach zero. Figure 10.21a shows the comparison of temperature distribution

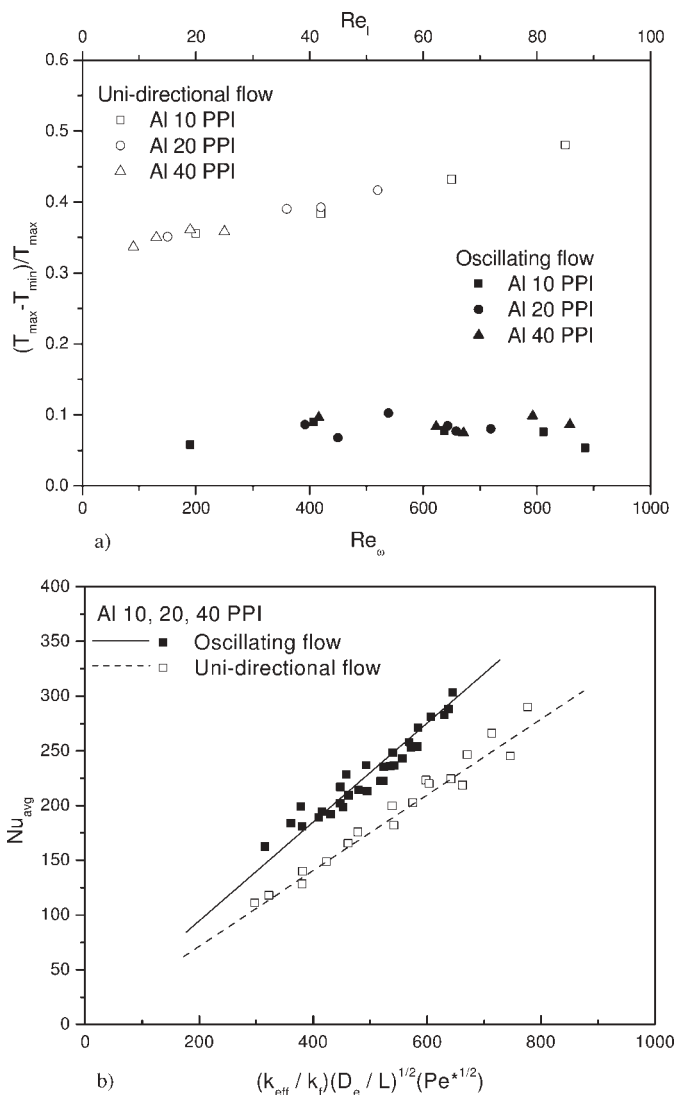


Figure 10.21 (a) Temperature uniformity in steady and oscillating flows; (b) grouping parameter $(k_{\text{eff}}/k_f)(D_e/L)^{1/2}Pe^{*1/2}$ as a function of length-averaged Nusselt number for oscillating and steady flows [59].

uniformity for steady and oscillating flows through aluminum foams of 10, 20 and 40 PPI. It is obvious that the ratio of the maximum temperature difference to the maximum local temperature on the surface for oscillating flow is much smaller than that for steady flow. According to data shown in Figure 10.21a, the average temperature uniformity index of oscillating flow is more than 6 times lower than that for steady flow. This indicates that the surface temperature distribution for oscillating

flow is more uniform than that for steady flow. Two thermal entrance regions of oscillating flow result in low temperature increases along the porous channel. To compare the heat transfer performance between the steady and oscillating flows through metal foam channel, the length-averaged Nusselt number is used to calculate the average local Nusselt number over the whole length of the test section. Based on the derivation of Eq. (10.41), the length-averaged Nusselt number can be expressed as

$$Nu_{avg} = C \left(\frac{k_{eff}}{k_f} \right) \left(\frac{D_e}{L} \right)^{1/2} (Pe^*)^{1/2} \quad (10.51)$$

where C is a constant which has been determined experimentally. As shown in Figure 10.21b, the length-averaged Nusselt numbers for steady and oscillating flows can be collapsed into two straight lines by employing the grouping parameter. It can be seen that the length-averaged Nusselt numbers for both oscillating and steady flows increase with the grouping parameter. The slope of the line for oscillating flow is larger than that for steady flow. The constants C obtained by the present study for steady and oscillating flows are 0.34 and 0.51, respectively. The larger value of constant C for oscillating flow shows that better heat transfer performance of oscillating flow through the metal foam channel can be obtained compared to steady flow. The ratio $Nu_{avg}(osc)/Nu_{avg}(std)$ shows that heat transfer rate for oscillating flow can be 1.5 times that for steady flow through aluminum foams. The presence of two thermal entrance regions at the test section with higher cycle-averaged local Nusselt number results in a higher length-averaged Nusselt number for oscillating flow.

For high-speed microprocessors, the reliability of transistors and their operating speeds are not only influenced by the average temperature but also by temperature uniformity on the substrate surface. The temperature of the hot spot can often affect calculated performance due to prolonged gate delay, and will always govern the overall reliability of the silicon. The results shown in Figure 10.22 indicate that oscillating flow through porous media is a potential cooling method to maintain a uniform on-die temperature distribution below certain limits.

10.4.2

Pumping Power of Oscillatory Cooling System

The required power for driving coolants through heat sinks is one of the concerns in actual thermal design. To evaluate the driven force in metal foam with different pore densities subjected to oscillating flow, the pumping power of the oscillatory cooling system needs to be analyzed together with the heat transfer performance. Figure 10.22a shows the variations of the measured maximum pressure drop and velocity with kinetic Reynolds number for oscillating flow through 10, 20 and 40 PPI aluminum foams. The data show that the maximum pressure drops and velocities increase with increasing kinetic Reynolds number, i.e. dimensionless oscillatory frequency. It can be seen that the maximum pressure drop for aluminum foam with high pore density is much higher than that for aluminum foam with low pore

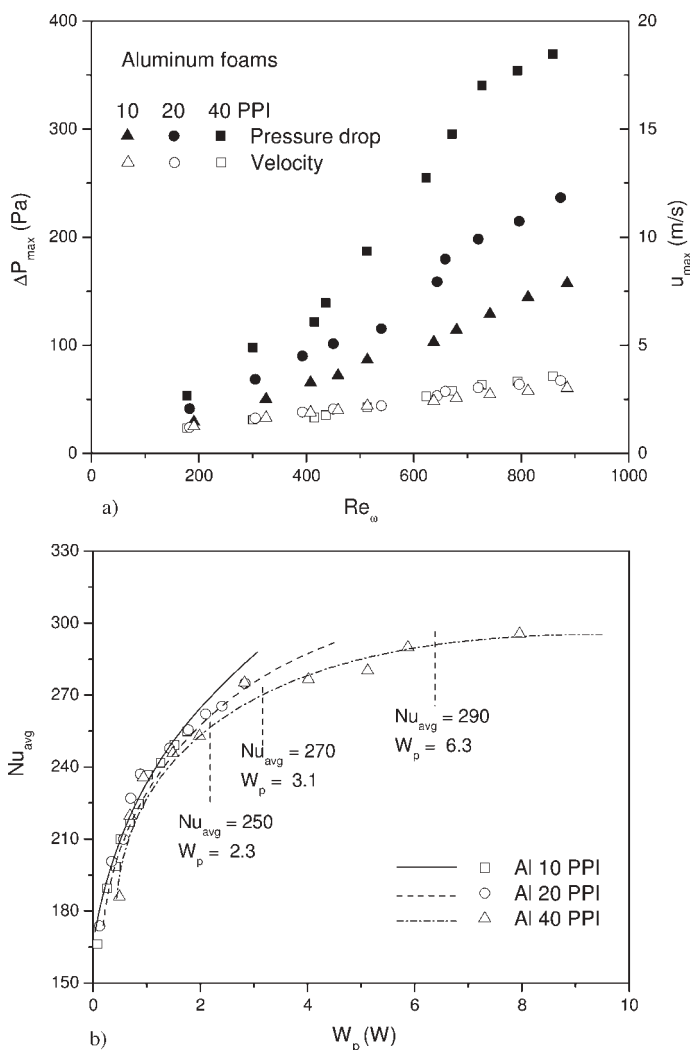


Figure 10.22 (a) Maximum pressure drop and velocity of oscillating flow through aluminum foams; (b) pumping power versus length-averaged Nusselt number for oscillation cooling system [59].

density while the increase of the maximum velocity with the kinetic Reynolds number is not as significant. This implies that the appropriate velocity for cooling electronic components can be obtained at a relative low pressure drop by using oscillating flow through an aluminum foam heat sink. Consequentially, a higher driven force is required in oscillating flow through high pore density foam in order to obtain the same flow velocity as compared to that required in low pore density foam due to the conservation of energy principle. In the design of heat sinks for

cooling electronic packages, the heat removal capability of the heat sink must be assessed together with the driven force required to operate the system, i.e. the pumping power. The required maximum pumping power for oscillating flow through metal foam heat sink is defined as

$$W_p = \Delta P_{\max} \dot{V} \quad (10.52)$$

where W_p and $\dot{V}$ are the average maximum pumping power and volumetric flow rate, respectively. The data for the maximum pumping power versus the length-averaged Nusselt number for oscillating flow through 10, 20 and 40 PPI aluminum foams are plotted in Figure 10.22b. It can be seen that the relationship between the maximum pumping power and length-averaged Nusselt number is nonlinear. The pumping power increases with the length-averaged Nusselt number of oscillating flow in aluminum foam with various pore densities. The data in Figure 10.22b show clearly that the large length-averaged Nusselt numbers of oscillating flow in 40 PPI aluminum are achieved at the expense of larger pumping power. The trend of fitting curves shows that the same length-averaged Nusselt number under small pumping power can be obtained by oscillating flow through aluminum foam with low pore density. It can also be observed that the increase of length-averaged Nusselt number at large pumping power is not significant, especially for high pore density aluminum foam. For example, with an increase in the average Nusselt number from 270 to 290 in 40 PPI aluminum, the pumping power is increased sharply from 3.1 to 6.3 W. At the same time, there is only a 1.3 times increase in pumping power when the average Nusselt number is increased from 250 to 270. This indicates that relatively high heat transfer performance can be obtained in low pore density metal foam subject to oscillating flow by an appropriate pumping power. The results suggest that in the design of a novel heat sink, metal foams of low pore density can be used to enhance heat transfer with low pumping power. High pore density metal foams with their extremely large fluid–solid contact surface areas and tortuous coolant flow paths are suitable to remove high heat fluxes in applications where pumping power is not of concern.

10.5

Conclusions

This chapter brings together a variety of analytical and experimental studies of fluid flow and heat transfer of oscillating and steady flows through open-cell metal foams. Salient results are summarized below:

1. Based on an analysis of similarity parameters, it is found that the characteristics of oscillating flow through metal foam channel are dominated by the flow parameters of oscillation frequency and maximum flow displacement for a porous channel with constant geometrical dimensions. The maximum friction factor of oscillating flow through aluminum foams was obtained in terms of the hydraulic

ligament diameter-based kinetic Reynolds number $Re_{\omega(Dh)}$ and the dimensionless flow amplitude A_{Dh} .

2. The pressure drop and velocity of oscillating flow in an open-cell metal foam increase with increasing oscillatory frequency and flow amplitude, and vary almost sinusoidally due to the reversing flow direction. The maximum pressure drop in high pore density metal foam is larger than that in low pore density metal foam. This indicates that for constant porosity, a high pore density aluminum foam corresponds to high flow resistance compared to low pore density aluminum foam. The analysis shows that the increase of flow resistance in metal foam is directly related to the effective surface length, which relates an increase in drag to the increase in specific surface area.
3. The local temperatures were found to decrease with an increase in the kinetic Reynolds number while the cycle-averaged local Nusselt numbers exhibit the opposite trend for oscillating flow through metal foam. The heat transfer performance of oscillating flow through an aluminum foam with constant properties is governed by the oscillatory frequency and flow displacement. The empirical correlation $Nu_{avg} = 12.38 A_0^{0.95} Re_{\omega}^{0.31}$ of the length-averaged Nusselt number shows that the effect of A_0 on the heat transfer behavior in oscillating flow is more dominant than that of Re_{ω} due to the larger exponent of A_0 . It implies that higher heat transfer performance can be obtained by oscillating flow through a porous channel with relatively low frequency and high displacement. For very high kinetic Reynolds number, the increase in heat transfer of oscillating flow through open-cell metal foam channel is marginal.
4. Based on the local thermal nonequilibrium model, the scale analysis shows that the dimensionless grouping parameter

$$\left(\frac{k_{eff}}{k_f}\right) \left(\frac{D_c}{L}\right)^{1/2} Pe^{*1/2}$$

is a function of the length-averaged Nusselt number. The comparison shows that the total heat transfer rates of oscillating flow can be 1.5 times larger than that of steady flow through a metal foam channel. The average temperature uniformity index I_{uni} of oscillating flow is more than 6 times lower than that for steady flow. This indicates that the surface temperature distribution for oscillating flow is more uniform than that for steady flow, due to the low temperature increases along the channel caused by two thermal entrance regions of oscillating flow.

5. The local thermal equilibrium condition of oscillating flow in porous media can be verified by the ratio of the time scale of the variation of the flow or thermal boundary condition to the time scale concerning the thermal inertia of the porous media. When the characteristic time $t_p = (1 - \varepsilon)(\rho_s C_{ps})/ha$ of the porous media is much shorter than the time scale $t_o = 1/\omega$ concerning the variation of the boundary condition, the local thermal equilibrium can be achieved and the temperature difference between the solid and fluid phases can be neglected.

6. The studies of thermal management by using metal foams show that heat transfer coefficients offered by open-cell metal foams are consistently higher than those offered by commercially available products. The thermal resistance of aluminum foam heat sinks displayed more than 28% reduction compared to conventional parallel-plate heat sinks. It can be concluded that metal foams with high thermal conductivity, large surface area-to-volume ratio and tortuous coolant flow path are preferred in the design of compact heat exchangers and heat sinks.
7. For an oscillatory cooling system, the heat transfer rate increases with the increase of the pore density at a constant kinetic Reynolds number, i.e. dimensionless oscillatory frequency. However, for a given pumping power, better heat transfer performance can be achieved by low pore density metal foam under the condition of oscillating flow. In designing a novel heat sink, metal foams of low pore density can be used to enhance heat transfer with small pumping power. High pore density metal foams with their extremely large fluid–solid contact surface areas and tortuous coolant flow paths are suitable to remove extraordinarily high heat fluxes in applications where pumping power is not of concern.

Nomenclature

a	specific surface area ($\text{m}^2 \text{m}^{-3}$)
A, B, C_1, C_2	variables
A_0	dimensionless flow displacement, $x_{\max}/D$
A_{Dh}	hydraulic ligament diameter-based dimensionless flow amplitude, $x_{\max}/D_{\text{h}}$
A_{p}	amplitude of pressure gradient (Pa)
Bi	Biot number, haH^2/k
c	form coefficient of porous media
C	constant
C_{D}	thermal dispersion coefficient
c_{p}	specific heat ($\text{J kg}^{-1} \text{K}^{-1}$)
d_{l}	ligament diameter of porous media (μm)
D	diameter of pipe (m)
Da	Darcy number, $\sqrt{K}/H$
D_{C}	form drag (N)
D_{e}	hydraulic diameter of the channel (m)
D_{h}	hydraulic ligament diameter of metal foam (m)
D_{μ}	viscous drag (N)
f	oscillatory frequency (Hz)
F	inertial coefficient of porous medium (m^{-1})
f_{max}	maximum friction factor of oscillating flow
f_{osc}	average friction factor of oscillating flow
F_{ω}	function of friction factor for oscillating flow,
	$\frac{\sqrt{C_1^2 + C_2^2}}{16\sqrt{\left(\frac{1}{2}\sqrt{Re_{\omega}} - 2C_1\right)^2 + 4C_2^2}}$

h	convective heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
H	height of the channel (m)
I_{uni}	temperature uniformity index, $(T_{\text{max}} - T_{\text{min}})/T_{\text{max}}$
k	thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
k_d	thermal dispersion conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
k_{eff}	effective thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
k_{se}	effective thermal conductivity of solid ($\text{W m}^{-1} \text{K}^{-1}$)
k_{fe}	effective thermal conductivity of fluid ($\text{W m}^{-1} \text{K}^{-1}$)
K	permeability of the porous medium (m^2)
L	length of the test section (m)
M	ratio defined in Eq. (10.45 a)
N	ratio defined in Eq. (10.45 b)
Nu_{avg}	average Nusselt number along the test section
Nu_s	average Nusselt number for the smooth plate
Nu_x	local Nusselt number, $h_x D_e / k_f$
P	pressure (Pa)
Pe_x^*	effective local Peclet number, ux/α^*
ΔP	pressure drop (Pa)
Q	power input (W)
Re_l	Reynolds number based on ligament diameter, ud_l/ν
Re_K	Reynolds number based on permeability, $u\sqrt{K}/\nu$
$Re_{\text{max(Dh)}}$	maximum hydraulic ligament diameter based Reynolds number, $A_{\text{Dh}} Re_{(\omega \text{ Dh})} / 2$
Re_{ω}	kinetic Reynolds number, $\omega D_e^2 / \nu$
$Re_{\omega(\text{Dh})}$	hydraulic ligament diameter based kinetic Reynolds number, $\omega D_h^2 / \nu$
R_{th}	thermal resistance (K W^{-1})
t	time (s)
t_0	time scale defined in Eq. (10.47)
t_p	time scale defined in Eq. (10.47)
T	temperature ($^{\circ}\text{C}$)
$\mathbf{u}$	velocity vector
u	flow velocity (m s^{-1})
U	dimensionless velocity
V_s	volume of solid fraction of metal foam (m^3)
V_t	total volume of metal foam (m^3)
$\dot{V}$	average maximum volumetric flow rate ($\text{m}^3 \text{s}^{-1}$)
W_p	maximum pumping power (W)
X	dimensionless horizontal coordinate
x_{max}	amplitude of flow displacement (m)
Y	dimensionless transverse coordinate

Greek

α^*	effective thermal diffusivity ($\text{m}^2 \text{s}^{-1}$)
δ	uncertainties
δ_t	thickness of thermal boundary layer (m)

ε	porosity of medium
θ	dimensionless temperature
μ	dynamic viscosity (N s m^{-2})
μ_e	effective fluid viscosity (N s m^{-2})
ν	kinematic viscosity ($\text{m}^2 \text{s}^{-1}$)
ρ	density (kg m^{-3})
τ	dimensionless time
ϕ	surface porosity
ω	angular frequency (rad s^{-1})

Subscripts

avg	average value
e	effective
f	fluid phase
fs	interface between fluid and solid phases
max	maximum
min	minimum
s	solid phase
x	local quantity

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11

Radiative and Conductive Thermal Properties of Foams

Dominique Baillis and Rémi Coquard

11.1

Introduction

During the last decade, solid foams have shown a strong development. Indeed, they permit a substantial improvement in the performance of standard materials in numerous technological fields. Among the different foams, it is possible to observe two types of foam: (1) open-cell foams and (2) closed-cell foams.

Metallic and ceramic open-cell foams exhibit thermal, mechanical and exchange properties that make them very interesting in many applications requiring multifunctionality. To illustrate this, we can cite a nonexhaustive list of functions for which they are usually used: ultralow-weight panels, energy-absorbing structures, heat dissipation media, electrodes for electric batteries, ultrasound deflectors, carrying structures for catalysts and heat exchangers.

Closed-cell foams have also found applications in a large number of technological fields. They are notably used for packaging or mechanical protection, due to their excellent mechanical resistance. However, thermal insulation is their main area of application. As a matter of fact, numerous materials used in frigorific or building insulation have a closed-cell structure. After glass wools, polystyrene or polyurethane foams are the most widely sold materials for building thermal insulation. For example, expanded polystyrene (EPS) foams represent more than 25% of the building insulation market in France. They are very convenient to manipulate due to their mechanical properties (lightness and stiffness) and they are relatively cheap.

In most of these applications, the knowledge and modeling of the thermal properties is of primary importance to improve the thermal performances. Thermal properties are greatly dependent on the type of foam associated with different cellular structure. Cellular foams generally present a low density, and thus the radiative heat transfer is significant.

11.2

Description of Cellular Foam Structure

The foam structure varies depending on whether they are open- or closed-cell foams.

11.2.1

Open-Cell Foams

Open-cell foams have a reticular structure. In this simplest case, the bulk material concentrates entirely on the cell sides shaping the struts. The interstitial gas is the same as the external environment gas, typically air. As an example, Figure 11.1 shows carbon and aluminum open-cell foams. The solid matrix is made of struts oriented in different directions in space. Note that the strut thickness is always much smaller than the cell diameter.

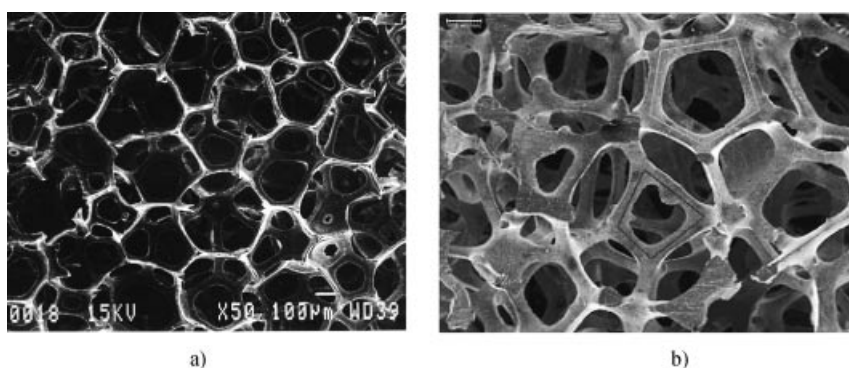


Figure 11.1 SEM images of open-cell foam cuts:
(a) open-cell carbon foam; (b) open-cell aluminum foam.

11.2.2

Closed-Cell Foams

Closed-cell foams are generally classified as cellular materials. Among the most usual closed-cell foams, polystyrene and polyurethane foams can be cited. The cells are delimited by thin membranes (walls). Walls intersect at cell edges where strut formation can occur or not depending on the type of closed-cell foam. EPS foams present only walls, whereas extruded polystyrene foams and polyurethane foams are formed by walls and struts.

EPS foams present a particular structure directly due to their production process. They are characterized by double-scale porosity. Indeed, as shown in Figure 11.2, the porous structure of EPS foams is composed of two different types of pores [1,2].

- From surface analysis, the expanded polystyrene structure appears as many pellets welded together (Figure 11.2a). Pores with irregular shape are formed by the free space between the pellets. The pore size varies from one to several millimeters and

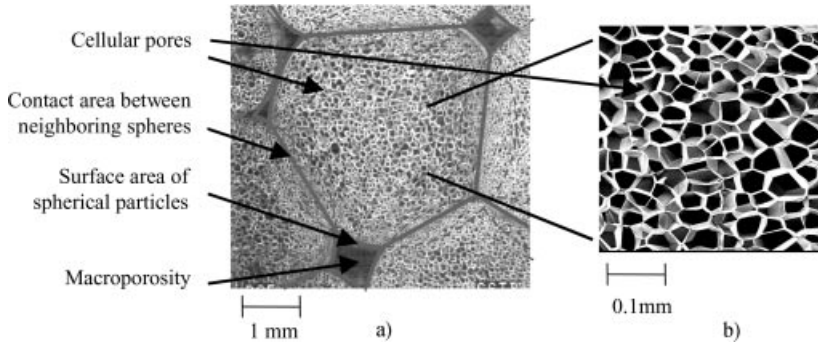


Figure 11.2 SEM images representing macro- and microporosity of EPS foams: (a) macroscopic structure; (b) cellular structure [1].

the average pellet's diameter varies from about 2 mm for a 35 kg m^{-3} foam to about 5 mm for a 10 kg m^{-3} foam. The porosity due to the interpellet space varies from 4 to 10% for standard EPS foams.

- Figure 11.2b shows the internal structure of a pellet portion magnified 100 times using scanning electron microscopy (SEM). Cellular pores are contained in the pellet. They are made only by walls that intersect at the cell sides without giving rise to bulk material agglomeration: there is no strut formation. The gas filling the pores is air. Moreover, the cell diameter is much larger than the wall thickness. The order of magnitude of the size of the pore contained in the beads is approximately $100 \mu\text{m}$. The porosity of the cellular medium contained in the pellets varies from 97 to 99.5%.

Extruded polystyrene (XPS) foams and polyurethane (PUR) foams have the most complex cellular structure with not only walls (cell faces) but also struts formed at the junction of the cells. As an example, Figure 11.3 shows an SEM image of a PUR foam. Walls are usually thinner than struts and cell diameter is much larger than strut thickness.

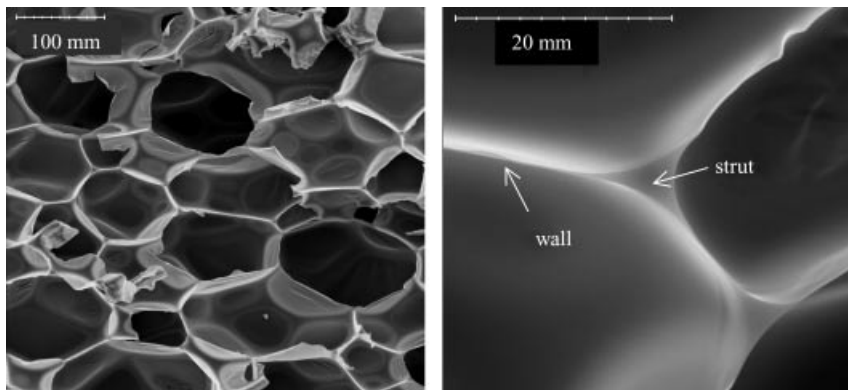


Figure 11.3 SEM images of PUR foam.

11.3

Modeling of Foam Structure

As we will see in the next section, the computation of the conductive and radiative thermal properties greatly depends on the modeling of the foam structure. More particularly, the radiative properties depend on shape and the number of particles by volume unit constituting the foam.

11.3.1

Cell Modeling

According to Reitz [3] a foam structure can be represented by polyhedral cells. Three usual shapes of polyhedral cells are shown in Figure 11.4: cubic cells (square faces), dodecahedral cells (pentagonal faces) and tetrakaidecahedral cells (square and hexagonal faces). The geometric properties of these three polyhedral cells are given in Table 11.1. Note that the type of polyhedral cell influences the number of struts by unit volume (which is an essential parameter to predict radiative properties).

Most of the papers in the literature that are based on microscopic analysis of different foams show that the unit cell of foams closely resembles a pentagon dodecahedron [4–9]:

- struts are formed by the intersection of three walls;
- four struts are connected to form intersection volume;
- most of the cell faces contain five struts, only a few contain four and six struts.

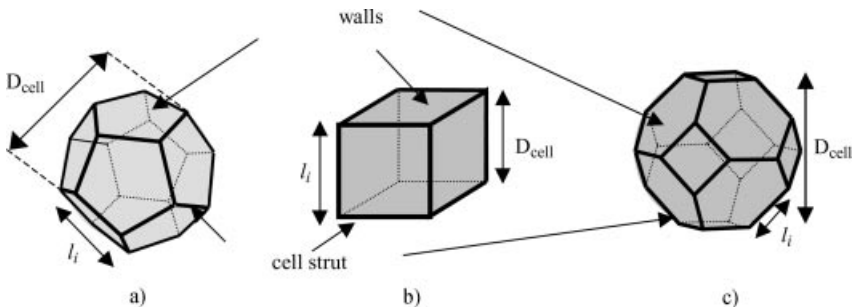


Figure 11.4 Three different shapes of polyhedron cellular structure: (a) pentagon dodecahedron; (b) cube; (c) tetrakaidecahedron.

Table 11.1 Geometric characteristics of three polyhedral cells.

Polyhedron	Diameter	Volume	Strut number/volume unit (N_v)
Cube	l_i	l_i^3	$4/l_i^3$
Pentagon dodecahedron	$2.57l_i$	$7.663l_i^3$	$1.305/l_i^3$
Tetrakaidecahedron	$2.995l_i$	$11.314l_i^3$	$1.061/l_i^3$

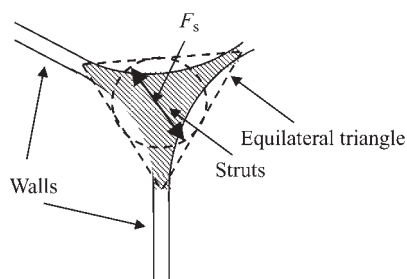


Figure 11.5 Cross-section through struts inscribed in an equilateral triangle.

11.3.2

Particle modeling

Foam structure is usually decomposed into simpler elements constituting particles interacting with radiation. Basing upon microscopic analysis of different foams, structure modeling usually consists in dividing cells into walls and struts. Walls and struts are modeled respectively like thin slabs (platelets) and cylinders. Platelet thickness is usually assumed to be the same as the mean wall thickness. Moreover, from microscopic analysis, it can be observed that the cross-section of struts formed at the junction of three cells is triangular incurved, concave (Figure 11.3). This cross-section seems to be inscribed in an equilateral triangle (Figures 11.3 and 11.5). Glicksman and Torpey [4] from SEM analysis have deduced that the fraction defined as the strut cross-sectional area to the equilateral triangle area is $f_s = 2/3$.

11.4

Determination of Foam Conductive Properties

The formulation of the heat conduction problem requires a single parameter k_c , usually called the “effective thermal conductivity”. This parameter expresses the magnitude of heat conduction in both solid and gas phases. Actually, this formulation, based on a unique parameter, uses the assumption of the equivalent homogeneous medium: that is to say, the conductive behavior of the two-phase materials could be accurately represented by that of an equivalent homogeneous conductive medium. This hypothesis is valid when the dimensions of the pores are very small compared to the external dimensions of the material. In the case of usual foams, these conditions are satisfied.

The effective conductivity k_c depends on the properties of the two different phases but also on the morphology of the material. For example, the magnitude of heat conduction could vary widely between two materials made of similar phases and with comparable porosities but having different microstructures. It is therefore particularly difficult to estimate the effective conductivity of solid foams due to the large difference encountered between the conductivity of the two phases and

to the complexity of the pore geometry. We can divide the studies into two categories according to the solution method used: analytical/semi-analytical and numerical models.

11.4.1

Analytical/Semi-analytical Models

In many usual solid foams, heat conduction is the main mode of heat transfer at ambient temperature, and thus the modeling of their effective conductivity has been the subject of numerous studies. Most of these works are based on empirical or analytical models. The analytical and semi-analytical models are generally based on the electrical analogy.

11.4.1.1 Polymer Foams

The first study was conducted by Schuetz and Glicksman [10,11]. These authors were interested in the conductivity of polymeric foams formed of closed or open cells. They considered that the foams are made of windows, occupying the faces of polyhedral cells, and/or cell struts located at the junction between the different faces. The porosity of these foams was above 95%. They modeled the foam as a network of thermal resistances and made several simplifications of the morphology. They studied the influence of the shape of the cells on the apparent conductivity by applying their computations to foams made of cubic cells or to random mixing of cell struts. They concluded that the porosity and the proportion of solid in struts are the only parameters influencing the apparent conductivity. Notably, they found that the shape and size of the cells and the shape of cell struts have no influence on this conductivity. Their analytical models based on the previous simplifications permit them to compute analytical overestimating (upper limit) and underestimating (lower limit) values of the exact conductivity. These values are related to the porosity, the conductivity of air and polymer and to a single morphological parameter (f_s) representing the fraction of solid phase in the struts. Finally, they proposed the following formula for the computation of the effective conductivity of polymeric foams:

$$k_c = \varepsilon k_{\text{fluid}} + (1 - \varepsilon) \left(\frac{2 - f_s}{3} \right) k_{\text{solid}} \quad (11.1)$$

The model indicates that the accumulation of the solid phase in the struts tends to diminish the heat conduction. Then, for given solid and fluid phases and for a given porosity, heat conduction is more important in closed-cell foams than in open-cell foams. The factor $(2 - f_s)/3$ can be explained intuitively by considering a cubic cell and the limiting cases $f_s = 0$ and $f_s = 1$. Indeed, when there is no accumulation of matter in the struts ($f_s = 0$), the entire polymer is comprised in the cell windows and a proportion of $2/3$ ($= (2 - 0)/3$) of the polymer is oriented in the direction of the heat flux. In contrast, when the entire polymer is present in the struts (open cells $f_s = 1$), this proportion is only $1/3$ ($= (2 - 1)/3$).

More recently, Leach [12] conducted a study in which he recapitulated the different analytical models used for the computation of the effective thermal conductivity of cellular media (parallel-series model, cubic model, spherical model). He showed that all of these models tend to a single expression for the effective conductivity in the form

$$k_c = \varepsilon k_{\text{fluid}} + k_{\text{solid}}(1-\varepsilon)\frac{2}{3}X \quad (11.2)$$

where X is a factor taking a value between 0 and 1. This formulation reinforces the formula proposed by Schuetz and Glicksman. As a matter of fact, the model of Schuetz and Glicksman is widely accepted and has been used by numerous authors. Actually, most of the studies dealing with the modeling of heat transfer in highly porous polymer foams (such as PSE, XPS or PUR foams) have used it. It has the advantages of great simplicity and relative accuracy for highly porous materials.

However, this model is based on a simplified representation of the foam microstructure. Moreover, the solution method uses the electrical analogy and the parallel-series network approximation. The limitations of this correlation led the researchers dealing with foams with higher solid fractions or with more specific microstructures to develop their own model.

Ahern *et al.* [13] studied experimentally the variation of the effective conductivity of PUR foams by subtracting the measured radiative conductivity to the equivalent conductivity obtained experimentally. They concluded that the model proposed by Glicksman and Schuetz [10,11] does not fully describe their experimental data especially at relatively high solid fractions. As expected, they explained these differences by the fact that basic assumptions of the model of Schuetz and Glicksman (small solid fraction and gas conductivity negligible when compared to the solid one) are not satisfied in PUR foams. They proposed a correction of the model that was first developed for the electrical conductivity of liquid foams and which predicts more correctly their experimental data. This correction is based on the Maxwell relation [14] for mixtures of materials of different (electrical) conductivities. This relation is generally applied to foams made of low or nonconducting spheres (the bubbles) in a well-conducting matrix (the solid phase), which is hard to justify in the case of solid foams as the gas phase takes up over 90% of the volume, in sharp contrast with the dilute limit assumed in the Maxwell derivation. Therefore, the authors considered that the gas phase is the background material and the solid phase is taken as the low-density dispersed phase. Although the geometry of the solid polymeric phase is certainly not described by spheres, it may be assumed that the struts are cylinders and the windows are plates. These considerations lead to

$$k_c = \frac{k_{\text{fluid}}\varepsilon + k_{\text{sol}}F(1-\varepsilon)}{\varepsilon + (1-\varepsilon)F} \approx k_{\text{fluid}} + (k_{\text{sol}} - k_{\text{fluid}})F(1-\varepsilon) + o((1-\varepsilon)^2) \quad (11.3)$$

where the last term is a linear expansion valid for small solid fractions.

The shape factor was volume averaged in terms of windows and struts as

$$F = (1 - f_s)F_{\text{window}} + f_s F_{\text{strut}} \quad (11.4)$$

A similar calculation to Maxwell's was used for spheres, which leads, for cylinders and platelets, to

$$F_{\text{strut}} = \frac{1}{3} \left(1 + \frac{4k_{\text{fluid}}}{k_{\text{fluid}} + k_{\text{sol}}} \right); \quad F_{\text{window}} = \frac{2}{3} \left(1 + \frac{k_{\text{fluid}}}{2k_{\text{sol}}} \right) \quad (11.5)$$

We note that if the gas conduction can be ignored ($k_{\text{fluid}} \rightarrow 0$) these shape factors reduce to the conventional values of $F_{\text{strut}} = 1/3$ and $F_{\text{window}} = 2/3$.

An excellent agreement with experimental results is obtained for low solid fractions but for larger solid fractions the prediction is less accurate. However, a serious step towards full quantitative agreement is achieved.

11.4.1.2 Ceramic, Metallic and Carbon Foams

Today, metallic, ceramic and carbon foams show a strong development in many applications due to their multifunctionality. Their thermal properties, notably their effective conductivity, have to be known with good accuracy. Moreover, due to the great difference between the thermal conductivities of the two phases encountered in such foams, the choice of the model used is even more important and should describe the cellular geometry accurately.

Fu *et al.* [15] studied theoretically the evolution of the thermal conductivity of ceramic foams. They represented the foam geometry from two different unit cell models: the first unit cell is a cubic-shaped box with square ligaments on the border of the box; the second unit cell is formed by a solid cube which is voided centrally. The effective thermal conductivity is calculated using the thermal-circuit method [16]. This method consists in dividing the unit cell into infinitesimal slices along the heat flux direction. The slices are assumed to be associated in series and their thermal resistance is calculated as if the solid and fluid phases were associated in parallel in each slice. They compared the results given by the two geometrical models with each other and with experimental data of the literature obtained for different porosities and at different temperatures.

Lu and Chen [17] modeled the thermal transport properties of aluminum alloy foams, which exhibit exceptional resistance to fire. The apparent thermal conductivities of two-dimensional foams having a variety of two-dimensional cellular microstructures are first calculated analytically. These include regular honeycombs, equilateral triangles, squares, closely packed circles, Voronoi structures and Johnson–Mehl models. For each of these structures, the authors estimated the thermal conductivity in the two orthogonal directions (x, y) as

$$k_{x,y} = C(1 - \epsilon)k_s \quad (11.6)$$

The authors only consider heat transport via solid conduction and assumed that the entire solid is present in struts of cells (no accumulation of matter at the junction

of two struts). Thereafter, the effects of several types of geometric imperfection (plateau borders, cell-edge misalignments, fractured cell edges, missing cells, inclusions and cell size variations) are studied by using analytical as well as finite element methods implemented in the ABAQUS software.

Calmidi and Mahajan [18] and Bhattacharya *et al.* [19] provided an analysis for estimating the effective thermal conductivity of high-porosity metal foams. They represented the open-cell structure by a model consisting of a two-dimensional array of hexagonal cells where fibers form the sides of the hexagon. The presence of lumps of metal at the junction of two fibers is taken into account by considering square [18] or circular [19] blobs of metal. They computed the effective conductivity of the medium by dividing the unit cell in several sections having a constant solid phase repartition and using the electrical analogy. The thermal conductivity of each section is obtained by assuming that the thermal resistances of the solid and fluid phases are associated in parallel. Whereas the thermal resistance of the entire unit cell is calculated by considering that the thermal resistances of each section are in series. Their theoretical results have been validated by experimental measurements on aluminum and reticulated vitreous carbon foams using air and water as fluid phases. The analysis shows that the porosity and the ratio of the cross-sections of the fibers and the fiber junctions strongly influence the results but that there is no systematic dependence on the size of the cells. According to the results of their model, they proposed an empirical correlation which is a linear combination of series and linear models:

$$k_c = A(\varepsilon k_f + (1-\varepsilon)k_s) + \frac{(1-A)}{\varepsilon/k_f + (1-\varepsilon)/k_s} \quad (11.7)$$

with a best-fitting value $A = 0.35$.

Boomsma and Poulikakos [20] also proposed an analytical effective thermal conductivity model of a saturated porous metal foam. Their structural representation is based on a three-dimensional cell geometry: the idealized basic tetrakaidecahedron. The foam is modeled as a network composed of cubical nodes placed on the vertex of the tetrakaidecahedron and circular cylindrical ligaments joining these nodes. They conducted a complete geometric analysis of the cellular morphology and expressed the porosity according to the dimensionless foam ligament radius and the dimensionless cubic node length. The method of solution of the conductive heat transfer is close to that used by Calmidi and Mahajan [18] and Bhattacharya *et al.* [19]. Indeed, the authors divided the three-dimensional unit cell in several layers in series, each layer containing solid and fluid phases in parallel. The layers are chosen, so that the repartition of solid and fluid phases is constant. They obtained an expression of the effective conductivity of the foam according to the previous dimensionless geometric parameters and of the thermal conductivities of each phase. They used the experimental data of Calmidi and Mahajan [18] to identify the values of the dimensionless geometric parameters and compared the results of their model to experimental results. They found good agreement with experimental measurements made on aluminum foams with air or water as the saturating fluid. They show that, despite

the high porosity of the foam, the heat conductivity of the solid phase controls the overall effective thermal conductivity to a large extent, and that an accurate representation of the contribution of the solid portion of the foam conductivity is needed in effective conductivity models.

11.4.2

Numerical Models

We can see that when analytical models are used, several approximations are required to simplify the method of solution. Notably, researchers always have recourse to the series-parallel network analogy. Moreover, the structure of the foam is idealized. For example, the cross-sections of the struts are always assumed circular or square and the accumulation of matter at the junction of several struts is always represented as cubes or spheres when they are considered. To improve the accuracy of the model, several studies had recourse to numerical simulations which take into account various morphologies of the cellular structure.

11.4.2.1 Polymer Foams

Saadatfar *et al.* [21] carried out a computational study of mechanical and thermal properties of polyester foams based on tomograms of a range of closed-cell polymeric foamed materials with porosities ranging from 40 to 75%. The cellular structure of these materials differ significantly from the cell geometry considered in the model of Schuetz and Glicksman as the porous material is close to an arrangement of air bubbles in a polymer matrix. Therefore, it is not surprising that the model of Glicksman is not suitable for these materials. The tomograph permits three-dimensional images of the pores to be obtained and taking into account very faithfully the real microstructure of these foams. Another advantage is that no assumption has to be made on the structure of the foams. To solve the conduction equation, the three-dimensional voxel microstructure is first converted into a network of thermal resistors by connecting each pair of adjacent voxels by a resistor. A potential gradient is then applied in each coordinate direction, and the system is relaxed using a conjugate gradient technique to evaluate the field. By this manner, it is possible to analyze the effective conductivity of the foam in the three Cartesian directions. It was found that the materials studied are practically isotropic and the average effective conductivities were compared with an equation of the form

$$k_c = k_{\text{sol}}(1-\varepsilon) + k_{\text{air}}\varepsilon \quad (11.8)$$

The fit of the numerical results to the empirical equation is excellent across the full range of porosity. Note that this correlation differs strongly from the model of Schuetz and Glicksman (Eq. 11.1) but this is not surprising given that we already underlined the fact that the microstructure of these polymeric foams with relatively low porosity is notably different from the microstructure assumed by Schuetz and Glicksman. This example demonstrates the interest in numerical models based on complex representations of the pore structure as it permits one to obtain simple

analytical relations predicting accurately the conductive properties of materials with a particular porous structure. The results show a potential for future development of more accurate correlations between structure and transport properties for real porous materials.

11.4.2.2 Ceramic, Metallic and Carbon Foams

Druma *et al.* [22] conducted a numerical finite element analysis to calculate the thermal conductivity of open- and closed-cell carbon foams with different levels of porosity ranging from 0 to 1. They considered a homogeneous dispersion of spherical voids ($k_{\text{fluid}} = 0$) in a solid matrix represented by a unit cell consisting of a cube with 1/8 spherical shape pores at each corner and one sphere in the middle of the cell. From this unit cell, they generated a microscopic scale finite element grid within the solid material of the foam. This finite element grid was implemented in the ALGOR finite element model (FEM) software. This software solves the steady-state heat conduction equation in a piece of foam sandwiched between two slabs of nonporous solid:

$$\vec{\nabla}(\vec{K}\vec{\nabla}T) = 0 \quad (11.9)$$

with the boundary conditions: $T = T_{\text{cold}}$ at the lower bottom face of the slab; $T = T_{\text{hot}}$ at the top face of the slab and $\partial T / \partial \vec{n} = 0$ on all other surfaces.

The software predicts the temperature and heat flux distribution in the piece of porous media and computes the corresponding effective conductivity from the relation

$$k_c = \frac{Q_k}{\Delta T / \Delta z} \quad (11.10)$$

Owing to the symmetry of the geometry of the unit cell used and in order to save time, the computations were carried out using only a set of cells in the vertical direction. Actually, the complete model for FEM analysis was constructed by repeating the unit cell ten times in the vertical direction.

Thereafter, they compared their results with the analytical approach developed by Bauer [23]. This approach leads to the following formula for the effective conductivity:

$$k_c = (1 - \varepsilon)^{1/n} k_{\text{sol}} \quad (11.11)$$

where n is a conduction parameter depending on the pore shape and pore concentration.

They determined the conduction parameter numerically for different porosity levels. It appears that the FEM solution matches the theoretical prediction at the low porosity level. But a 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

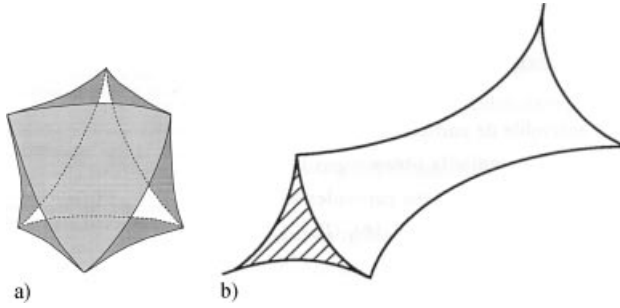


Figure 11.6 Carbon foam particles.

accurately predict the thermal conductivity of foams over the full range of porosity. The value of this parameter increased from the theoretical value of 0.67 at low porosity, to approximately 0.83 at 90% porosity.

Coquard and Baillis [24] developed a FEM of conduction transport in highly porous open-cell foams in order to calculate the effective thermal conductivity of different ceramic or metallic foams. The porosity of the materials varies from 75 to 100%. The foam cellular microstructure is modeled by various polyhedral open cells formed by solid struts with different shapes.

From photographs of several metal foams obtained using SEM, they remarked that the cell windows are not always pentagonal but that square or hexagonal windows are also present. They concluded that the morphology of real foams could not be described exactly using a single cell shape (generally pentagonal dodecahedrons) but that it is actually composed of several types of cells close to dodecahedron, cube and tetrakaidecahedron. Therefore, in order to investigate the influence of the cell's shape on the conductive properties of the foam, their model could take into account ideal foams composed of cubic, dodecahedral or tetrakaidcahedral cells.

With regard to the cell struts, from the SEM images and an analysis of tomographic images, Coquard and Baillis noticed that they are close to triangular cylinder whose cross-section is concave. They also observed that the cross-section is not constant along the length of the struts but that the struts are thicker at their tips. The real struts could be faithfully represented by the scheme of Figure 11.6. However, those authors modeled struts with simpler cross-sections and they investigated the influence of the strut cross-section on the conductive properties. They simulated full or hollow struts with square or triangular constant cross-sections.

Their numerical FEM simulates the three-dimensional steady-state heat transfer in a slab of foam with two perfectly insulated sides, sandwiched between two slabs of nonporous solid maintained at temperatures T_{cold} and T_{hot} . The steady-state heat conduction, Eq. (11.9), is solved in Cartesian coordinates:

$$\frac{\partial}{\partial x} \left(k_{x,y,z} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{x,y,z} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_{x,y,z} \frac{\partial T}{\partial z} \right) = 0 \quad (11.12 \text{ a})$$

$$T|_{z=0} = T_{\text{cold}}; \quad T|_{z=Z} = T_{\text{hot}} \quad (11.12 \text{ b})$$

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = \left. \frac{\partial T}{\partial x} \right|_{x=X} = 0; \quad \left. \frac{\partial T}{\partial y} \right|_{y=0} = \left. \frac{\partial T}{\partial y} \right|_{y=Y} = 0 \quad (11.12 \text{ c})$$

The model uses an iterative process and a spatial discretization dividing the foam slab into $nX \times nY \times nZ$ cubic elementary volumes made of solid or gas phases with different conductivities (k_{solid} for solid nodes and k_{fluid} for fluid nodes), which reproduces the foam microstructure.

The numerical results obtained confirm several conclusions drawn by the previous studies, notably concerning the strong influence of the solid fraction and the solid conductivity and the neutrality of the cell diameter.

11.5

Determination of Cellular Foam Radiative Properties

For low-density foam such as usual open- and closed-cell foams (described in Section 11.2), radiative heat transfer is significant. The radiative properties of foams required for solving the radiative transfer equation are more complex than the conductive properties. Indeed, there are three parameters instead of one, and each of these parameters is a function of the wavelength of the thermal radiation. The three parameters are the spectral volumetric scattering and absorption coefficients, and the spectral phase function. The main difficulty in predicting heat transfer in foam material is the determination of radiative properties. There are two main groups of methods used to determine the radiative properties of porous media: (a) prediction models (such as the well-known Mie theory) and (b) experimental methods based on parameter identification techniques. Baillis and Sacadura [25] made a review of the different studies devoted to the modeling and measurement of the radiative properties of porous media.

- Little work has been done on the prediction of radiative properties from foam microstructure and porosity. Foam radiative properties are difficult to model due to their complex structure but these models are very powerful as they permit the understanding of the complex physical radiative phenomena occurring in the foam. This microscopic approach applied to open-cell foam structure was followed by Baillis *et al.* [9] for carbon foam and more recently by Loretz *et al.* [26] for metallic foam. Other authors [1,2,6,7] modeled radiative properties of closed-cell foam such as polystyrene and polyurethane foams.
- There are some works on the determination of radiative of foams using the parameter identification method. We can cite, as examples, the works of Skocypec *et al.* [27], Hale and Bohn [28] and Hendricks and Howell [29] on reticulated ceramics and those of Kuhn *et al.* [7] and Baillis and Sacadura [30] on polystyrene and polyurethane foams. Two types of transmittance and reflectance measurements are usually used: directional-hemispherical or directional-directional. Extinction

and scattering coefficients are identified by assuming an isotropic phase function, a phase function of Henyey and Greenstein or a combination of different phase functions.

Before we describe and discuss the models proposed in the literature to predict cellular foam radiative properties, a summary of the theoretical basis for general particulate media is necessary.

11.5.1

Theoretical Prediction of Radiative Properties of Particulate Media

In order to predict the radiative transfer in particulate media, it is necessary to know how the particles individually interact with incident radiation upon them.

11.5.1.1 Single-Particle Properties

The question concerning the interaction of radiation with a particle can be solved by considering a plane, monochromatic wave incident upon a particle of a given shape, size and optical constants ($\tilde{n} = n - ik$), and by applying Maxwell's equations. This has been done for spheres, cylinders and spheroids. Solutions to these various problems such as the well-known Mie theory may be found in standard texts on electromagnetic scattering theory [31–33], or on radiative heat transfer [34–36]. These solutions provide the fundamental radiative properties for particle emission, absorption and scattering, which are the extinction efficiency Q_e , the albedo ω and the phase function $p(\theta)$. The extinction coefficient Q_e is the ratio of the extinction cross-section, C_e , of the particle to the geometrical cross-section G . The albedo is the ratio of the scattering efficiency (or cross-section) of the particle to the extinction efficiency (or cross-section):

$$Q_e = \frac{C_e}{G}; \quad \omega = \frac{Q_s}{Q_e} \quad (11.13)$$

The most commonly used solution is the Mie theory. Before considering the full Mie solution, it is useful to examine some limiting regions where simpler analytic results apply. These limiting regions are defined by the magnitude of the particle size parameter x ($x = \pi D/\lambda$, where D is the particle diameter and λ the wavelength) and the optical constants $\tilde{n} = n - ik$ [34]. Each of these limiting regions is described by expressions that are simpler than those for the full Mie theory (more details can be found elsewhere [34]):

- if $x \ll 1$ and $x|\tilde{n}-1| \ll 1$, the limiting solution of the Mie theory is known as Rayleigh scattering;
- if $x \gg 1$ and $x|\tilde{n}-1| \gg 1$, geometric optics (ray tracing) and diffraction theory can be used to predict the scattering behavior;

- if $|\tilde{n}-1| \ll 1$ and $x|\tilde{n}-1| \ll 1$, the limiting solution, referred to as Rayleigh–Gans scattering, applies;
- $x \gg 1$ and $x|\tilde{n}-1| \ll 1$, the limiting behavior, referred to as anomalous diffraction by van de Hulst, is obtained.

11.5.1.2 Dispersion Properties

The particle radiative properties that are required for integration of the radiative transfer equation are the extinction coefficient, albedo and phase function. They are derived for an optically thin, differential volume of space occupied by many particles of possibly different sizes and shapes. They can be obtained from the radiative properties of single particles by adding up the effects of all the particles of different sizes and shapes [34]:

$$\beta = \sum_i C_{e,i} N_i; \quad \sigma = \sum_i C_{s,i} N_i; \quad \omega = \frac{\sigma}{\beta}; \quad P = \frac{1}{\sigma} \sum_i C_{s,i} P_i N_i \quad (11.14)$$

where N_i is the number of particles of type i per unit volume.

Note that for randomly oriented particles, the characteristics must be averaged over all the possible directions of the incident:

$$C_{e,i} = Q_e \bar{G}_i; \quad C_{s,i} = Q_s \bar{G}_i \quad (11.15)$$

where $\bar{G}_i$ is the average geometrical cross sectional area of a particle of type i .

As a result, radiative properties can be obtained from morphological data (such as particles shape or number of particles, etc.) and optical properties of the solid matrix. Some data can be difficult to obtain directly and can be determined from the parameter identification method.

11.5.2

Parameter Identification Method

The parameter identification method is very useful. Indeed, it can be used not only to determine the extinction coefficient, scattering coefficient and phase function parameters (as discussed above at the beginning of Section 11.5) but also to obtain unknown data required in the prediction model of radiative properties.

The parameter identification method uses:

- experimental data of transmittances and reflectances (T_{ei}) obtained in several measurement directions (i), for a given set of samples;
- theoretical transmittances and reflectances (T_{ti}) calculated for the same directions as the ones of the experimental data and for the same sample thickness.

Two approaches can be used depending on the unknown parameters:

- If all the parameters are function of wavelength (such as radiative properties), for each wavelength the goal is to determine the parameters $p_1, p_2, \dots, p_n$, which

minimize the quadratic relative differences (D) between the measured and calculated transmittances over the N measurements:

$$D(p_1, \dots, p_n) = \sum_{i=1}^N [T_{ti}(p_1, \dots, p_n) - T_{ei}]^2 \quad (11.16)$$

- If some parameters are not functions of wavelength (such as morphological parameters), it is not necessary to carry out the identification process for each wavelength and the process can occur only one time. Thus the goal is to determine the parameters $p_1, p_2, \dots, p_n$, which minimize the quadratic relative differences (D) between the measured and calculated transmittances over the N measurements and NW measurements wavelengths:

$$D(p_1, \dots, p_n) = \sum_{j=1}^{NW} \sum_{i=1}^N [T_{tij}(p_1, \dots, p_n) - T_{eij}]^2 \quad (11.17)$$

Different types of measurements can be performed inducing a different number of measurements N in the identification process:

- directional-hemispherical measurements: $N=2$ (one for hemispherical transmittance and one for hemispherical reflectance measurements);
- directional-directional measurements: $N=N_{bd}$, where N_{bd} is the total number of bi-directional measurement directions;
- combination of directional-directional and directional-hemispherical measurements: $N=2+N_{bd}$.

Several techniques can be used in the identification process. As an example, we can cite the Gauss linearization method [37] which minimizes D by setting to zero the derivatives with respect to each of the unknown parameters.

The bi-directional transmittances or reflectances $T(\mu)$ for normal incidence are defined by the following expression:

$$T(\mu) = \frac{I(\mu)}{I_0 d\omega_0} \quad (11.18)$$

where I is the transmitted or reflected intensity and I_0 the intensity of the collimated beam normally incident onto the sample within a solid angle $d\omega_0$.

The hemispherical transmittances or reflectances are defined by the following expressions:

$$T(\mu) = 2\pi \frac{\int_0^1 I(\mu) \mu d\mu}{I_0 d\omega_0} \quad (11.19 a)$$

$$R(\mu) = -2\pi \frac{\int_{-1}^0 I(\mu) \mu d\mu}{I_0 d\omega_0} \quad (11.19 b)$$

11.5.3

Application to Open-Cell and Closed-Cell Foams

As we have seen in Section 2, the different types of cellular foam with open or closed cells present different structures composed of different particles. As a result, for each type of foam the models must be adapted to take into account the particle shapes and sizes.

11.5.3.1 Open-Cell Carbon Foam

Starting from microscopic analysis, Doermann and Sacadura [38] and Baillis *et al.* [9] have considered that open-cell carbon foams are composed of two types of particles: struts with varying thickness and strut junctures (Figures 11.6 and 11.7). As four struts are connected at each strut juncture, if N_1 is the number of struts per unit volume, there are $N_1/2$ strut junctures per unit volume.

The particles are assumed to be opaque. Moreover, they are assumed to have a random orientation in the calculation of the average geometrical cross-sectional area of particles ($\bar{G}_i$). The scattering phenomena are accounted for by applying a combination of geometric optics and diffraction theory to these particles. Indeed, as the particle size parameter x is much larger than unity and the refractive index $\tilde{n}$ is not too small ($x|\tilde{n}-1| \gg 1$), geometric optics combined with diffraction theory can be used to predict scattering behavior. Moreover, due to the extremely large values of the diffraction phase function in the forward direction ($\theta \approx 0^\circ$), the diffraction contribution can be usually ignored [34] and treated as transmission.

For all large particles, if diffraction is neglected, the expressions for the efficiency coefficients are [32,35]

$$Q_e = 1; \quad Q_a = 1 - \rho_\lambda - \tau_\lambda; \quad Q_s = \rho_\lambda + \tau_\lambda \quad (11.20)$$

In these equations, ρ_λ represents the fraction of incident energy reflected at the front surface of the particle (the surface facing the collimated incident radiation), and τ_λ represents the fraction of incident energy that is transmitted into the particle.

The application of geometric optics laws to the two types of particles considered (particles of type 1 are struts, particles of type 2 are strut junctures) leads to the following results [39]:

$$\beta_\lambda = N_1(\bar{G}_1 + \bar{G}_2); \quad \sigma_\lambda = \rho_\lambda N_1(\bar{G}_1 + \bar{G}_2); \quad \alpha_\lambda = (1 - \rho_\lambda)N_1(\bar{G}_1 + \bar{G}_2) \quad (11.21)$$

The phase function corresponding to reflection from large opaque reflecting convex particles with random orientations can be adopted by applying the following *theorem* [32]:

The scattering pattern caused by a reflection on a very large convex particle with random orientation is identical to the scattering pattern by reflection on a very large sphere of the same material and surface condition.

For an open-cell carbon foam, Baillis *et al.* [39] assumed that the reflection is diffuse. The phase function related to reflection from large opaque diffusely reflecting sphere is [34]

$$P_r(\theta) = \frac{8}{3\pi}(\sin\theta - \theta\cos\theta) \quad (11.22)$$

Consequently the radiative properties can be determined from the parameters ρ_λ , N_1 , $\bar{G}_j$, $j = 1, 2$. Baillis *et al.* [39] have determined $\bar{G}_j$ as a function of the porosity ε and of the minimum and maximum thickness of the struts, b and $b_{\max}$. Moreover, by assuming that the foam cells have a regular pentagonal dodecahedron shape, the authors have also determined N_1 , as a function of the porosity ε , of the minimum and maximum thickness of the strut, b and $b_{\max}$, and of the parameter f_s .

Note that the parameters b , $b_{\max}$ and ε can be easily determined from microscopic analysis and images (Figure 11.7). The minimum and maximum thickness of the strut can be more precisely measured and are easier to obtain than the mean cell diameter. This is an advantage of this particle modeling which takes into account the varying thickness of the struts. The hemispherical reflectivity of the solid matrix, ρ_λ , cannot be obtained from direct measurement given that the material should be compacted for this measurement. Moreover, it cannot be obtained reliably from the literature because of the great dispersion of the reported data. So, Baillis *et al.* [39] have determined ρ_λ and f_s using an identification method.

For the carbon foam studied by Baillis *et al.* [39], the porosity measured is $\varepsilon = 98.75\%$ and particle dimensions obtained from a microscopic analysis are $b = 34 \mu\text{m}$, $b_{\max} = 52 \mu\text{m}$. The average values of the hemispherical reflectivity of carbon plus or minus the mean square deviation are presented in Figure 11.8. The radiative properties of the foam calculated from the prediction model are shown in

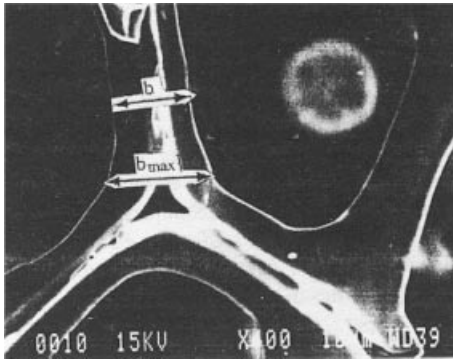


Figure 11.7 Microscopic analysis obtained from a carbon foam sample (magnification $\times 400$). Determination of dimensions b and $b_{\max}$ [39].

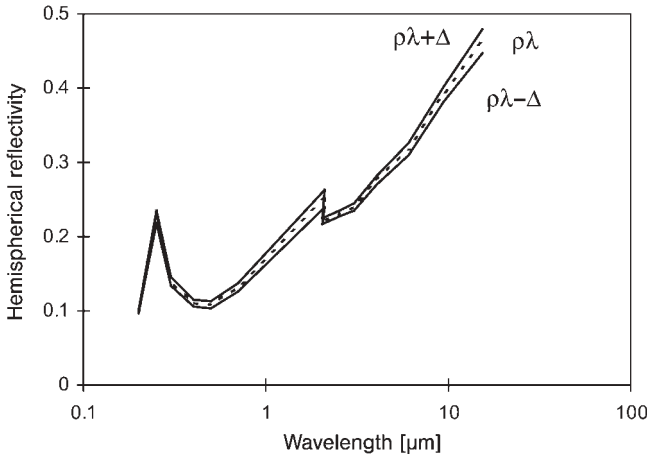


Figure 11.8 Identified carbon hemispherical reflectivity plus or minus the standard deviation ($\rho_\lambda \pm \Delta$) [39].

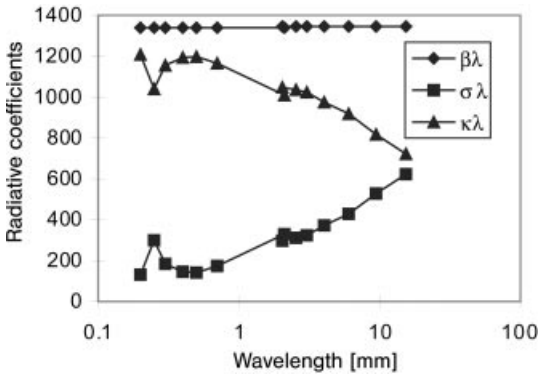


Figure 11.9 Radiative coefficients of a carbon foam [39].

Figure 11.9. Note that for visible wavelengths, the scattering coefficient is much smaller than the absorption coefficient due to the small reflectivity of carbon in the visible range. For higher wavelengths, the scattering coefficient increases.

11.5.3.2 Metallic Foam

The works of Loretz *et al.* [26] on aluminum open-cell foam are also based on geometric optics laws. Since the foam is metallic, the particles are assumed to be opaque. The scattering is thus limited to the reflection, and the hemispherical reflectivity ρ_λ is equal to the scattering albedo (Eq. (11.21)). The authors assume that the foam presents an intermediate reflecting behavior comprised between diffuse and specular reflection.

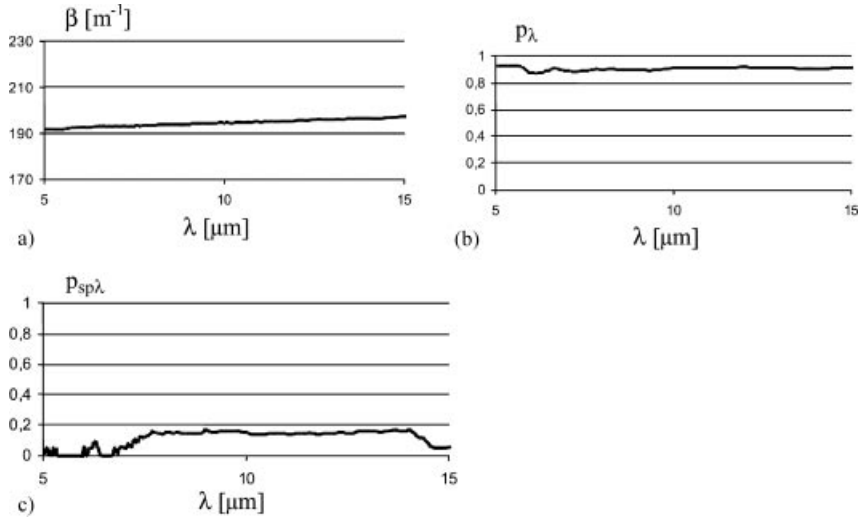


Figure 11.10 Radiative coefficients of an aluminum foam [26]:
(a) extinction coefficient; (b) aluminum hemispherical reflectivity;
(c) parameter of specularity.

Thus, the phase function is represented by a parameter which depends on the specularity. It will be called the parameter of specularity and denoted by $p_{sp\lambda}$. A value of zero for $p_{sp\lambda}$ corresponds to the diffuse reflection, whereas when $p_{sp\lambda} = 1$ the scattering is specular. An identification method for each wavelength is used to determine the extinction coefficient, the hemispherical reflectivity and the parameter of specularity from transmittances and reflectances measurements obtained using a Fourier transform infrared spectrometer. The results obtained for an aluminum open-cell foam of porosity 93% with particle dimensions $b = 0.58 \text{ mm}$, $b_{\text{max}} = 0.70 \text{ mm}$ are shown in Figure 11.10.

It can be observed that the extinction coefficient is almost independent of the wavelength. This confirms that geometrical optics can be applied to determine the radiative characteristics of the foam. The reflectivity is relatively important, 90% on average, which is logical considering the strong reflective ability of metallic matter. Finally, the parameter of specularity is close to zero for most of the wavelengths. It tends to confirm that the aluminum foam has a scattering behavior close to that of an opaque sphere with diffuse reflection. This assumption was used by Baillis *et al.* [39] in the case of carbon foams with open pores.

11.5.3.3 Closed-Cell Foam: Case of Low-Density EPS Foams

In the case of EPS foams, Coquard *et al.* [40] have shown that the macroscopic porosities (Figure 11.2) have practically no influence on the radiative properties. Thus, these properties could be obtained assuming that the porous morphology could be represented by a homogeneous cellular structure made exclusively of cell walls.

Regarding the shape of the cells, we have seen that they are generally represented as pentagonal dodecahedrons. However, the analysis of SEM images shows that, in real EPS foams, the cells forming the porous medium in the beads are not rigorously dodecahedrons but have rather irregular and random shapes composed of pentagonal, quadrilateral or hexagonal faces. Thus, their shape could not be perfectly described from a unique cell model but is more likely a combination of cubic, dodecahedral and tetrakaidecahedral cells. In order to investigate the influence of the morphology of cellular medium on the radiative properties of EPS foams, Coquard *et al.* [40] modeled these three different shapes. For each shape, the equation relating the diameter of the cells D_{cell} , the porosity ε and the thickness of the walls h is different. Indeed, we have the following.

- For dodecahedral cells: each cell is composed of 12 identical pentagonal faces, each of these walls being shared with one neighboring cell; there are finally 6 windows for one cell and then

$$(1-\varepsilon) = \frac{6 \times S_{\text{pentagon}} \times h}{V_{\text{dode}}} \Leftrightarrow h \approx 0.289 \times (1-\varepsilon) \times D_{\text{cell}} \quad (11.23)$$

- For cubic cells: each cell is composed of 6 identical square faces, each of these walls being shared with one neighboring cell; there are finally 3 windows for one cell and then

$$(1-\varepsilon) = \frac{3 \times S_{\text{square}} \times h}{V_{\text{cube}}} \Leftrightarrow h = \frac{(1-\varepsilon) \times D_{\text{cell}}}{3} \quad (11.24)$$

- For tetrakaidecahedral cells: each cell is composed of 6 identical square faces and 8 identical hexagonal faces, each of these walls being shared with one neighboring cell; there are finally 3 square windows and 4 hexagonal windows for one cell and then

$$(1-\varepsilon) = \frac{(3 \times S_{\text{square}} + 4 \times S_{\text{hexagon}})h}{V_{\text{tetra}}} \Leftrightarrow h \approx 0.299 \times (1-\varepsilon) \times D_{\text{cell}} \quad (11.25)$$

The mean diameter of the cells contained in EPS beads is generally between 100 and 300 μm , and then the height of the walls is greater than 100 μm , whereas the infrared radiation wavelengths at the origin of the radiative heat transfer at ambient temperature are close to 10 μm . Thus, the geometric optics and diffraction approximation could be used to treat the radiation/matter interaction for the particles considered. Furthermore, the influence of diffraction on the radiative heat transfer can be neglected. When the geometric optics approximation is valid and the diffraction neglected, the absorption and scattering cross-sections are computed by multiplying the cross-section of the particle by its absorptivity and reflectivity

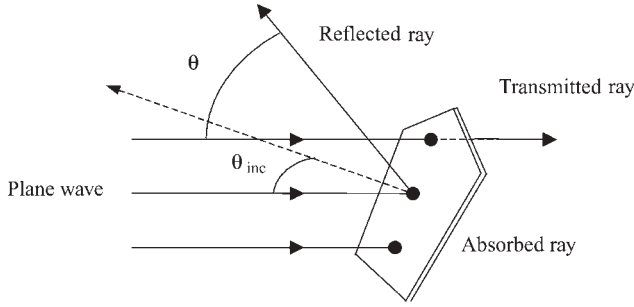


Figure 11.11 Interaction of a plane wave with a cell wall.

calculated by the Fresnel relations. The particles forming the cellular material are assumed to be randomly oriented; their radiative characteristics are averaged over all the possible directions of the incident wave:

$$\begin{aligned} \kappa_{\text{cell}} &= \sum_i N_i \times \bar{C}_{a,\lambda,i}; & \sigma_{\text{cell}} &= \sum_i N_i \times \bar{C}_{s,\lambda,i}; \\ \beta_{\text{cell}} &= \kappa_{\text{cell}} + \sigma_{\text{cell}}; & \phi_{\text{cell}}(\theta) &= \bar{\phi}(\theta) \end{aligned} \quad (11.26)$$

where N_i is the number of particles of type i per unit volume of cellular medium.

To compute these properties, Coquard *et al.* [40] used geometric optics laws, illustrated in Figure 11.11 for pentagonal windows. Windows are illuminated by rays representing the plane wave.

For dodecahedral cells, there are 6 pentagonal faces per cell and then

$$N_{\text{part}} = \frac{6}{V_{\text{cell}}} \approx \frac{14.06}{D_{\text{cell}}^3} \quad (11.27)$$

For cubic cells, there are 3 square faces per cell and then

$$N_{\text{part}} = \frac{3}{V_{\text{cell}}} = \frac{3}{D_{\text{cell}}^3} \quad (11.28)$$

For tetrakaidecahedral cells, there are 4 hexagonal faces and 3 square faces per cell and then

$$N_{\text{part},1} = \frac{4}{V_{\text{cell}}} \approx \frac{9.497}{D_{\text{cell}}^3} \quad \text{and} \quad N_{\text{part},2} = \frac{3}{V_{\text{cell}}} \approx \frac{7.123}{D_{\text{cell}}^3} \quad (11.29)$$

The computation of C_a and C_s is carried out from the reflectance R_{win} and the transmittance Tr_{win} of a thin slab using the thin-film optic laws stemming from the Fresnel relations and which take into account the interference effects. For dielectrics like polystyrene, we have

$$R_{\text{win}} = |r_{\text{win}}|^2; \quad Tr_{\text{win}} = |tr_{\text{win}}|^2 \quad (11.30.a)$$

$$\begin{aligned} r_{\text{win}} &= r_{12} + t_{12}r_{21}t_{21}e^{-i \times 2\hat{\beta}} + t_{12}r_{21}^3t_{21}e^{-i \times 4\hat{\beta}} \\ &+ \dots = \frac{r_{12} + r_{21}e^{-i \times 2\hat{\beta}}}{1 + r_{12}r_{21}e^{-i \times 2\hat{\beta}}} \end{aligned} \quad (11.30.b)$$

$$tr_{\text{win}} = t_{12}t_{21}e^{-i \times \hat{\beta}} + t_{12}r_{21}^2t_{21}e^{-i \times 3\hat{\beta}} + \dots = \frac{t_{12}t_{21}e^{-i \times \hat{\beta}}}{1 + r_{12}r_{21}e^{-i \times 2\hat{\beta}}} \quad (11.30.c)$$

where

$$\begin{aligned} \hat{\beta} &= \frac{2\pi \times \tilde{n} \times h \times \cos(\theta_{\text{ref}})}{\lambda}; \quad \sin(\theta_{\text{ref}}) = \frac{\sin(\theta_{\text{inc}})}{n}; \quad r_{12} = \frac{(|r_{12//}| + |r_{12\perp}|)}{2} \\ &= r_{21}; \quad t_{12} = 1 - r_{12} = t_{21}; \quad r_{12//} = \frac{n\cos(\theta_{\text{inc}}) - \cos(\theta_{\text{ref}})}{n\cos(\theta_{\text{inc}}) + \cos(\theta_{\text{ref}})} \quad \text{and} \quad r_{12\perp} \\ &= \frac{\cos(\theta_{\text{inc}}) - n\cos(\theta_{\text{ref}})}{\cos(\theta_{\text{inc}}) + n\cos(\theta_{\text{ref}})} \end{aligned}$$

To carry out the computation of R_{win} , and Tr_{win} the complex refractive index $\tilde{n} = n - ik$ of the polystyrene used in EPS foams has to be known. The variations of its real and imaginary parts obtained by the authors are shown in Figure 11.12 for the wavelength range 2–25 μm .

The variations of the extinction coefficient β_λ and the albedo $\omega_\lambda = \sigma_\lambda/\beta_\lambda$ with the radiation wavelength for cellular materials are illustrated in Figure 11.13 for the three different cellular shapes, for 0.99 porosity and for $D_{\text{cell}} = 200 \mu\text{m}$. As regards the scattering phase function, Figure 11.14 shows the phase function obtained

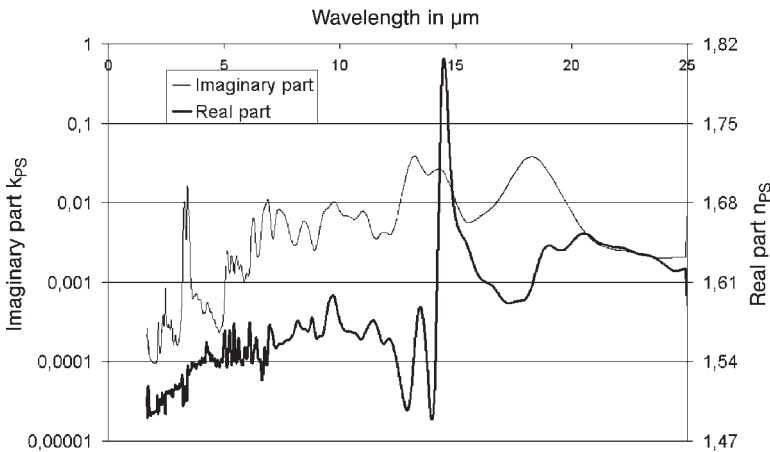


Figure 11.12 Spectral complex refractive index of polystyrene [1].

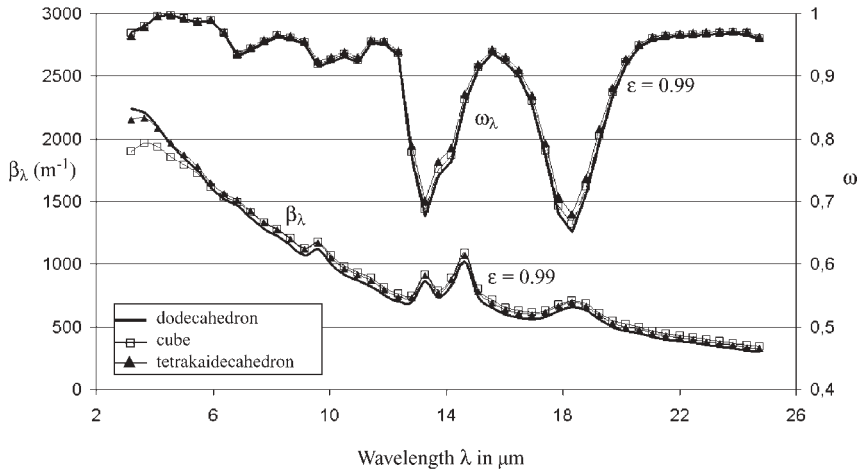


Figure 11.13 Theoretical variations of the extinction coefficient and albedo of EPS foams with the radiation wavelength for $D_{\text{cell}} = 200 \mu\text{m}$.

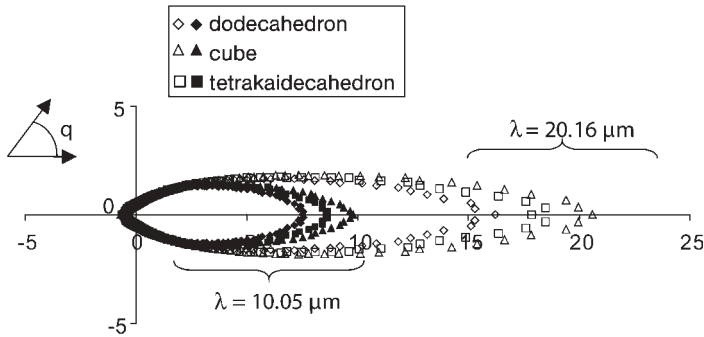


Figure 11.14 Theoretical phase function of an EPS foam with $D_{\text{cell}} = 200 \mu\text{m}$ and $\varepsilon = 0.99$ for the wavelengths $\lambda = 10.05$ and $20.16 \mu\text{m}$.

theoretically for the wavelengths $\lambda = 10.05$ and $20.16 \mu\text{m}$ with the three different cellular shapes in the case $D_{\text{cell}} = 200 \mu\text{m}$ and $\varepsilon = 0.99$. The variations of the asymmetric factor of the phase function

$$\langle \cos \theta \rangle = 0.5 \times \int_0^\pi P(\theta) \cos \theta \sin \theta d\theta$$

are depicted in Figure 11.15. This parameter permits us to characterize the repartition of the radiant intensity scattered by the medium. When $\langle \cos \theta \rangle > 0$, the radiation is preferentially scattered in the forward hemisphere and inversely. The results of the

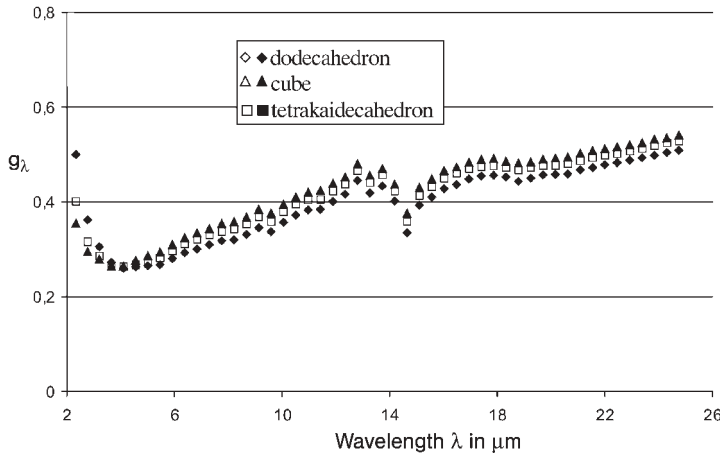


Figure 11.15 Variations of the asymmetry factor of the phase function with the radiation wavelength for EPS foams with $D_{\text{cell}} = 200 \mu\text{m}$ and $\varepsilon = 0.99$.

model presented show that in EPS foams, the radiation/matter interaction is dominated by scattering given that ω_λ is generally close to unity except for some wavelengths belonging to a polystyrene absorption peak. Moreover, we remark that the extinction coefficient is globally inclined to decrease with the wavelength, except for the wavelengths belonging to a polystyrene absorption peak. This tendency is entirely due to the morphological structure of EPS foams. Finally, we observe that the variations of the absorption and scattering coefficient are practically identical for the three polyhedral cells considered. Actually, the shape of the cells modeled only has a very slight influence on the behavior of the cellular material and, in practice, there is no need to characterize exactly the shape of the porous structure.

Concerning the scattering phase functions of EPS foams, Figure 11.14 shows that they are primarily oriented in the forward hemisphere whatever the wavelength. The radiant energy is predominantly scattered in a direction close to the incident direction. The graphs of Figure 11.15 also indicate that g_λ is inclined to increase with the wavelength. Moreover, as for the extinction and scattering coefficients, the shape of the cells considered has practically no influence on the repartition of the scattered energy.

11.5.3.4 Closed-Cell Foam: Case of XPS and PUR Foams

For XPS and PUR foams, the struts and walls are simultaneously present. Glicksman and Torpey [4] modeled polyurethane foam structure as a set of randomly oriented opaque struts, assuming an efficiency factor of one and neglecting scattering by struts. The strut cross-section was constant, triangular and occupied two-thirds of the area of an equilateral triangle formed at the vertices. The cell membranes within the foam are so thin (approximately $1 \mu\text{m}$) that they are assumed to be virtually transparent to thermal radiation. According to those workers, the struts, which constitute

approximately 85% of the solid polymer within the foam, are much thicker than the cell membranes and are responsible for most of the attenuation of thermal radiation. The foam cells are assumed to be pentagon dodecahedron cells. The resulting extinction coefficient is a simple function of the cell diameter and the foam porosity:

$$\beta = 4.09 \frac{\sqrt{1-\varepsilon}}{D_{\text{cell}}} \quad (11.31)$$

Kuhn *et al.* [7] adopted another geometrical model for the morphological structure of XPS and PUR foams. They assumed infinitely long randomly oriented cylinders to describe the struts and infinitely large platelets to describe the walls. The triangular cross-sections were converted into circular ones with the same geometric mean cross-section. Mie theory and geometric optics were used to describe the interaction of radiation with cylinders and platelets respectively. Under the independent scattering hypothesis, the foam extinction coefficient is obtained by adding up the effects of the two geometrical structures weighted by the strut fraction [32]:

$$\beta_{\lambda} = (1-f_s)\beta_{\lambda,\text{walls}} + f_s\beta_{\lambda,\text{struts}} \quad (11.32)$$

The foam cells are taken as regular pentagonal dodecahedrons. Placido *et al.* [2] used a similar model for PUR and XPS foams. They investigated the dependence of the radiative and conductive conductivities on geometrical parameters characterizing the internal foam structure, such as the mean wall thickness and the mean strut and cell diameters. The complex refractive index $\tilde{n} = n - ik$ of the polyurethane used in their calculations is obtained from the literature and is shown in Figure 11.16. Some results obtained will be discussed in Section 6.3. Details on the Mie theory applied to long cylinders can be found in Refs. [31,32]. Moreover, the model based on geometric optics to predict radiative properties of platelets has already been described in the case of EPS foams (containing walls only), and thus no additional details are given here.

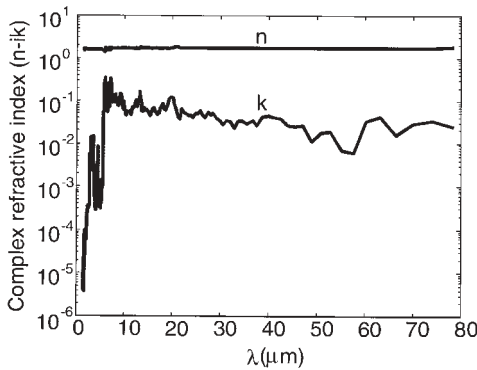


Figure 11.16 Spectral complex refractive index of polyurethane [2].

11.6

Combined Conductive and Radiative Heat Transfer in Foam

11.6.1

Heat Transfer Equations for Cellular Foam Insulation

Cellular foams are usually highly porous materials (with porosity larger than 80%). Heat transfer in such media occurs by conduction through the solid matrix and through the gas filling the pores, and by thermal radiation through the medium.

From a radiative point of view, foams are semitransparent media, as the walls and/or the struts absorb, emit and scatter radiation. Free convection can be neglected due to the small cell size.

For one-dimensional steady-state heat transfer, the energy equation is the following:

$$\frac{\delta q_c}{\delta z} + \frac{\delta q_r}{\delta z} = 0 \quad (11.33)$$

Assuming that the foam is a continuum medium, the conductive heat transfer follows the Fourier law. Thus, the conductive flux is related to the temperature by the relation

$$q_c = -k_c \frac{\delta T}{\delta z} \quad \text{and} \quad \frac{\delta q_c}{\delta z} = -k_c \frac{\delta^2 T}{\delta z^2} - \frac{\delta k_c}{\delta z} \frac{\delta T}{\delta z} \approx -k_c \frac{\delta^2 T}{\delta z^2} \quad (11.34)$$

The energy equation can be reformulated as

$$k_c \frac{\delta^2 T}{\delta z^2} = \frac{\delta q_r}{\delta z} \quad (11.35)$$

Radiative heat transfer in a low-density porous medium is a relatively complex problem given that it takes into account the emission, absorption but also the scattering of radiation by the porous material. The radiative heat transfer is described by an integrodifferential equation governing the spatial and angular distribution of monochromatic radiation intensity $I_\lambda(z, \mu)$ in the medium. For one-dimensional heat transfer with azimuthal symmetry the radiative transfer equation (RTE) is expressed as

$$\mu \frac{\delta I_\lambda(z, \mu)}{\delta z} = -\beta_\lambda I_\lambda(z, \mu) + \kappa_\lambda I_\lambda^0(T) + \frac{\sigma_\lambda}{2} \int_{-1}^1 \phi_\lambda(\mu' \rightarrow \mu) I_\lambda(z, \mu') d\mu' \quad (11.36)$$

and the boundary conditions for opaque diffusely reflecting boundaries are

$$\left. \begin{aligned} I_\lambda(0, \mu > 0) &= E_{\text{hot}, \lambda} I_\lambda^0(T_c) + 2(1 - E_{\text{hot}, \lambda}) \int_0^1 I(0, -\mu') \mu' d\mu' \\ I_\lambda(l, \mu < 0) &= E_{\text{cold}, \lambda} I_\lambda^0(T_f) + 2(1 - E_{\text{cold}, \lambda}) \int_0^1 I(l, \mu') \mu' d\mu' \end{aligned} \right\} \quad (11.37)$$

where E is the boundary emissivity. Parameters σ_λ , κ_λ and $\beta_\lambda = \sigma_\lambda + \kappa_\lambda$ characterize the ability of the medium to scatter, absorb and attenuate the radiation with wavelength λ . $\Phi_\lambda(\mu_{\text{inc}} \rightarrow \mu_{\text{sca}})$ characterizes the probability, for a radiation incident from an elementary solid angle around the direction with directing cosine $\mu_{\text{inc}} = \cos \theta_{\text{inc}}$, to be scattered in an elementary solid angle around the direction $\mu_{\text{sca}} = \cos \theta_{\text{sca}}$.

11.6.2

Resolution of the Heat Transfer Equations

To solve the conduction–radiation coupling, it is necessary to solve the radiative heat transfer problem.

11.6.2.1 Resolution of the Radiative Transfer Equation/Rosseland Approximation

Foams are usually thick enough to be considered as optically thick. So the radiative flux can be approximated by the Rosseland diffusive equation introducing a radiative conductivity, K_r (note that many works on foams used the Rosseland approximation [2,6,7,38]):

$$q_r = -k_r \frac{\delta T}{\delta z} \quad (11.38)$$

where

$$k_r = \frac{16n^2\bar{\sigma}T^3}{3\beta_R} \quad (11.39)$$

in which $\bar{\sigma}$ is the Stefan–Boltzmann constant and n is the effective index of refraction. It can be taken that $n = 1$ since the foam porosity is usually very high. Parameter β_R is the Rosseland mean extinction coefficient calculated over the entire wavelength range by the following relation:

$$\frac{1}{\beta_R} = \int_0^\infty \frac{1}{\beta_\lambda^*} \frac{\partial e_{b\lambda}}{\partial e_b} d\lambda \quad (11.40)$$

where e_b is the blackbody radiative emissive power.

The Rosseland approximation is valid when the medium absorbs and scatters isotropically. To take into account the foam anisotropic scattering, a weighted spectral extinction coefficient, β_λ^* , is used:

$$\beta_\lambda^* = \kappa_\lambda + \sigma_\lambda^* \quad \text{with} \quad \sigma_\lambda^* = \sigma_\lambda(1 - \langle \cos \theta \rangle_\lambda),$$

$$\langle \cos \theta \rangle_\lambda = 0.5 \int_{-1}^1 P_\lambda(\theta) \cos \theta d(\cos \theta) \quad (11.41)$$

As a result, the total conductivity includes the three independent mechanisms: conduction through the gas and through the solid material forming the cell, and thermal radiation [2,6,7,38]:

$$k_t = k_c + k_r \quad (11.42)$$

where $k_c = k_{c,\text{gas}} + k_{c,\text{sol}}$

11.6.2.2 Resolution of the Radiative Transfer Equation/Discrete Ordinates Method

Some foams, notably EPS foams with very low density, are not optically thick media and the Rosseland approximation is no longer valid [1]. Then the radiative heat flux cannot be related to the temperature distribution by the simple expression of Eq. (11.38). It is thus necessary to solve the radiative transfer equation (RTE).

Several numerical methods can be used to solve the RTE. For examples, we can cite the spherical harmonics method, the zone method of HOTTEL or the ray-tracing methods. The discrete ordinates method (DOM) is the most frequently used and gives accurate results. Coquard and Baillis [1] used it to solve radiative heat transfer in EPS foam.

The DOM is based on a spatial discretization of the slab thickness and an angular discretization of all directions. The angular discretization permits the replacing of the angular integrals by finite summations over N_d discrete directions with given weighting factors w . The spatial discretization must be the same as the one used for the numerical resolution of the energy equation. The accuracy of the results is strongly dependent on the angular discretization. Note that Coquard and Baillis [1] chose a very fine discretization dividing the 2π radians in 180 directions of 1° and whose weighting factors are proportional to the solid angle they encompass.

The RTE has to be solved for the entire wavelength range and the radiative heat flux divergence distribution is computed by integrating the contributions of each wavelength:

$$\frac{\delta q_r}{\delta z}(z) = \int_0^\infty \kappa_\lambda \left[4\pi I_\lambda^0(z) - 2\pi \sum_{j=1}^{N_d} I_{\lambda,j}(z) w_j \right] d\lambda \quad (11.43)$$

where the subscript j refers to the j th discrete direction.

In practice, to limit computational time and memory requirements, the spectral integration is made by considering that the intensity field in the slab is constant in N wavelengths bands covering the entire wavelengths. Then we have

$$\frac{\delta q_r}{\delta z}(z) = \sum_{i=1}^N \kappa_i \left[4\pi I_i^0(z) - 2\pi \sum_{j=1}^{N_d} I_{i,j}(z) w_j \right] \Delta\lambda_i \quad (11.44)$$

where the subscript i refers to the i th band and $\Delta\lambda_i$ is the width of the i th band.

11.6.2.3 Resolution of the Energy Equation

The total conductivities of foams can be calculated at sample mean temperature using Eq. (11.42) as in the works of Placido *et al.* [2]. However, to calculate the temperature distribution or the total heat flux in the foam sample, the energy equation can be solved numerically by an iterative process using the control volume method as in the works of Doermann and Sacadura [38] and Coquard and Baillis [1]. The principle of the control volume method is to divide the slab thickness into elementary control volumes [41]. The temperature of the medium at the center of each volume has to be calculated. The iterative process goes on as follows. First, an initial temperature distribution in the medium is chosen, for example linearly dependent on the z coordinates. Using this initial temperature distribution, the radiative problem is solved and the radiative heat flux divergence $\delta q_r / \delta z$ is calculated in each control volume. A new temperature distribution is then calculated from this heat flux divergence distribution in order to satisfy the energy equation (Eq. (11.33)). From this new temperature distribution, the radiative problem is solved again, a new radiative heat flux divergence distribution is calculated, and so on. The previous process is repeated until the difference between the temperature distribution obtained for two successive iterations is lower than a very small value synonymous with convergence. The total heat flux passing through the slab can then be computed in each control volume by adding the conductive and radiative heat flux. The “equivalent thermal conductivity” can be deduced.

11.6.3

Equivalent Thermal Conductivity Results

In order to quantify the total heat transfer passing through a slab of foam, one generally uses a parameter called the “equivalent thermal conductivity” or “total conductivity”, denoted by k_{equ} . Actually, it corresponds to the conductivity of the purely conductive material, which would lead to the same total heat flux under the same thermal boundary conditions. It is simply obtained by dividing the total heat flux density passing through a slab of materials by the temperature gradient, as if the heat transfer was purely conductive (Fourier law):

$$\phi = -k_{\text{equ}} \frac{\partial T}{\partial z}$$

To illustrate the contributions of each modes of heat transfer, the models presented in the previous paragraphs have been applied to compute the conductive and radiative properties of the different types of foams. The radiation–conduction coupling was then solved to obtain the variations of their equivalent thermal conductivities k_{equ} . As an example, some results are shown to underline the influence of morphological parameters or temperature on the thermal performances of some usual foams.

11.6.3.1 Closed-Cell EPS Foams

The model for determining the radiative properties presented in Section 5.3.3 has been used for several fictive EPS foams with different values of the structural

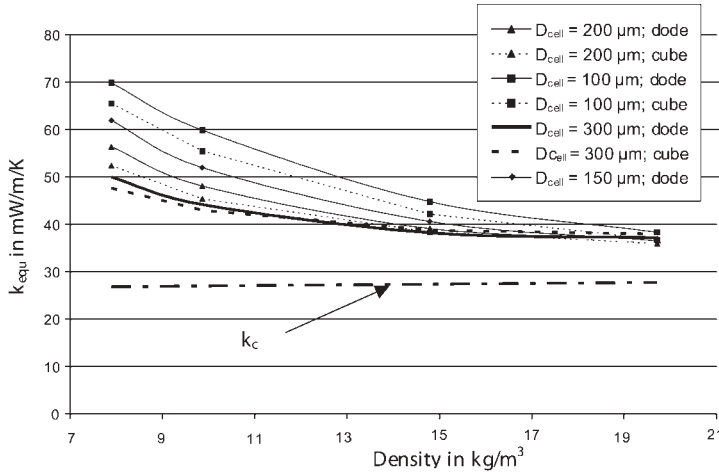


Figure 11.17 Evolution of the equivalent conductivity with the density for different mean cell diameter [1].

characteristics such as densities (ρ_{EPS}) and cell diameter (D_{cell}) covering the whole ranges of variation observed for usual EPS foams [1]. The effective phonic conductivity k_c of the EPS foams has been calculated using Eq. (11.1) proposed by Schuetz and Glicksman [10] with a proportion of polymer in the struts $f_s = 0$. The other parameters used for the computations are values commonly encountered in guarded hot-plate measurements: the mean temperature of the boundaries is $T = 296$ K ($T_{hot} = 304$ K and $T_{cold} = 288$ K); the slab thickness is equal to 40 mm; and the emissivities $E_{hot,\lambda}$ and $E_{cold,\lambda}$ of the hot and cold boundaries are gray and equal to 0.9. The discrete ordinates method is used to solve the radiative transfer equation. The energy equation is numerically solved using the control volume method discussed in Section 6.2.3.

Influence of the Foam Density The evolution of the equivalent thermal conductivity with the foam density is depicted in Figure 11.17 for foams with different mean cell diameters D_{cell} . The results obtained with the hypothesis of dodecahedral cells are referenced as “dode” whereas those obtained for cubic cells are noted “cube”. For clarity purposes, we have not represented the results obtained for tetrakaidecahedral cells as they are comprised between those obtained for cubic and dodecahedral cells and they do not bring any additional information. Also represented on the same figure is the evolution of the effective thermal conductivity k_c in order to illustrate the relative contributions of conduction and radiation to the total heat transfer. This effective thermal conductivity only depends on the density of the material.

The results show that the foam density has a strong influence on the equivalent conductivity of low-density EPS foams whatever the size and the shape of the cells. The lighter the foam is, the poorer is its thermal performance. This conclusion is well known in the building insulation industry for which often one has to find a compromise between light (and cheap) but weakly effective insulating materials and

a heavier (and more expensive) but more effective one. One can also remark that, due to the very high porosity of the material, the effective thermal conductivity k_c of the foam only increases imperceptibly and stays close to the thermal conductivity of air. Then, it reveals that the increase of the equivalent conductivity of EPS foams with decreasing density is entirely due to an increase of the radiant energy propagating through the medium. This could be intuitively explained by the fact that when foam gets lighter, the particles preventing the radiation from propagating in the medium are less opaque and the radiation/matter interaction is less pronounced. Radiative heat transfer then becomes relatively important and could represent more than 50% of the total flux passing through the slab for foams lighter than 10 kg m^{-3} . Moreover, as the effective phonic conductivity of EPS foams varies only very slightly with the density, we can conclude that all the variations of the equivalent conductivity k_{equ} with the different parameters are only due to variations of the radiative contribution.

The decrease of k_{equ} with increasing density is not linear and is more rapid for very light foams. One can also notice that the influence of the shape of the cells is non-negligible given that the equivalent conductivities stemming from the cubic cells assumption are lower than those obtained considering dodecahedral cells. This is due to the difference between Eqs. (11.23) and (11.27), and Eqs. (11.24) and (11.28), which are valid for dodecahedral and cubic cells respectively. However, the relative difference for the equivalent thermal conductivity is always lower than 7%.

Influence of the Mean Cell Diameter The theoretical results obtained using the same parameters as those presented above are now depicted in Figure 11.18 in order to show the influence of the mean cell diameter on the thermal performances of the EPS foams.

As can be noticed, the diameter of the cells forming the cellular medium contained in the beads also has a substantial influence on the equivalent thermal conductivity of the EPS foam. However, the variations of k_{equ} with D_{cell} are not the

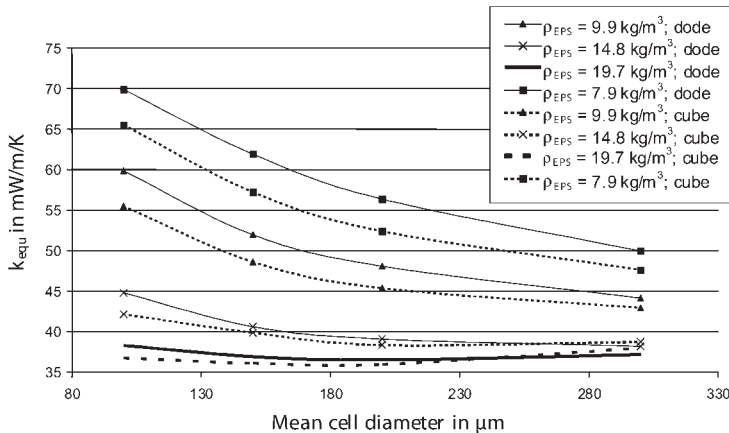


Figure 11.18 Evolution of the equivalent conductivity with the mean cell diameter for different porosities [1].

same for foams with different densities. Then, for very low-density EPS foams ($\rho_{\text{EPS}} < 10 \text{ kg m}^{-3}$), the results show that in the range of cell diameter studied ($100 \mu\text{m} < D_{\text{cell}} < 300 \mu\text{m}$), the equivalent conductivity decreases rapidly when D_{cell} increases. For example, for EPS foams of approximately 8 kg m^{-3} , the theoretical equivalent conductivity varies from 65 to $48 \text{ mW m}^{-1} \text{ K}^{-1}$ when the cell diameter goes from 100 to $300 \mu\text{m}$. We can also remark that the decrease of k_{equ} is slower when the cells are large.

When the density of the foam is greater than a fixed value, we can notice that there is an optimal cell diameter lower than $300 \mu\text{m}$ for which the equivalent conductivity of the foam slab is minimal. This optimal cell size depends on the foam density as well as on the morphology of the cell considered. Then, for foams of 14.8 and 19.7 kg m^{-3} in density, the optimal cell diameter is approximately 300 and $200 \mu\text{m}$ for dodecahedral cells and 250 and $200 \mu\text{m}$ for cubic cells. Actually, there is an optimal cell size whatever the density of the foam, but for very light foams this diameter is very large and greater than the diameter commonly observed in commercial EPS foams.

11.6.3.2 Closed-Cell XPS and PUR Foams

The model for determining the radiative properties presented in Section 11.5.3.4 has been used for several XPS and PUR foams with different densities, mean cell diameters and strut diameters [2]. The effective phonic conductivity k_c of the XPS and PUR foams have been calculated using Eq. (11.1) proposed by Schuetz and Glicksman [10]. The equivalent thermal conductivity is calculated using Rosseland approximation and Eq. (11.42) at mean temperature of 300 K .

Influence of the Foam Density Figures 11.19 and 11.20 show the curves of equivalent thermal conductivity, radiative conductivity, gas conductivity and solid conduc-

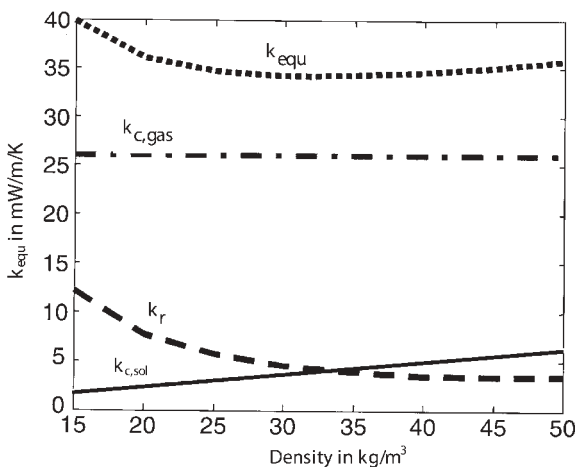


Figure 11.19 Equivalent thermal conductivity of XPS foams versus foam density (at 300 K , for $110 \mu\text{m}$ cell diameter and $2 \mu\text{m}$ strut diameter) [2].

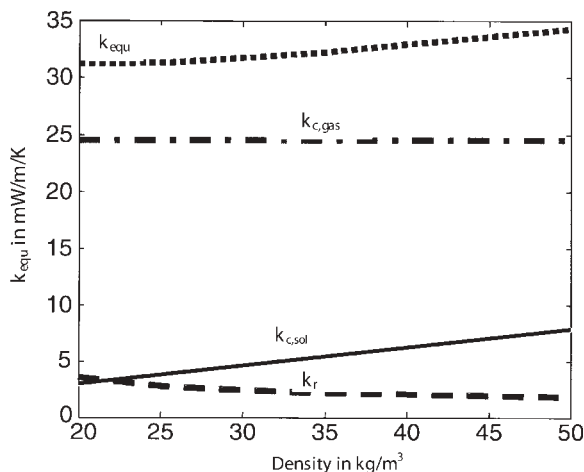


Figure 11.20 Equivalent thermal conductivity of PUR foams versus foam density (at 300 K, for 150 μm cell diameter and 2.5 μm strut diameter) [2].

tivity of XPS and PUR foams respectively versus foam density for a given cell and strut diameter. Note that the phonic conductivity is the sum of the gas conductivity and solid conductivity. It can be observed that the solid conductivity has a linear trend, whereas the gas conductivity is always constant. The equivalent total conductivity presents a minimum value due to the decreasing trend of the radiative conductivity and to the increasing trend of the solid conductivity.

Influence of the Mean Cell Diameter Figures 11.21 and 11.22 show the curves of the equivalent thermal conductivity, the radiative conductivity, the gas conductivity and the solid conductivity of XPS and PUR foams respectively as a function of the mean cell diameter for a given density. It can be observed that the solid conductivity and gas conductivity are almost constant. Thus, the minimum of equivalent total conductivity corresponds to the minimum of radiative conductivity. Note that the magnitude of the calculated total conductivity is in good agreement with measured data.

11.6.3.3 Metallic Open-Cell Foams

For metallic foams, we have seen particles are opaque to radiation and that the geometric optics assumption is valid. As a consequence, their radiative properties only depend on the morphology of the cellular structure, on the reflectivity of the solid phase and on the parameter of specularity $p_{sp\lambda}$ introduced by Loretz *et al.* [26]. In order to simplify the problem, the results illustrated have been obtained with the model used by these authors assuming that the cells have a dodecahedron shape, that the struts have a constant triangular cross-section and that there is no accumulation of matter at the junction of two struts.

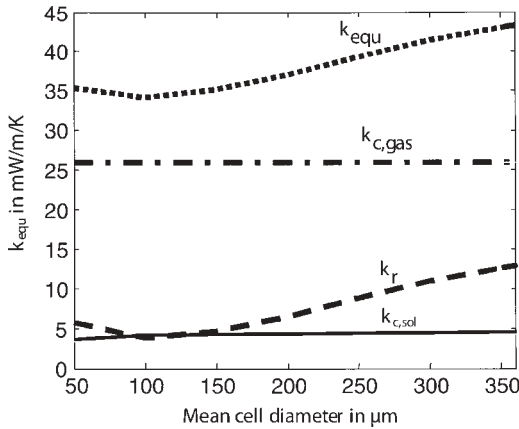


Figure 11.21 Equivalent thermal conductivity of XPS foams versus cell diameter (at 300 K, for 35 kg m^{-3} foam density and $2 \mu\text{m}$ strut diameter) [2].

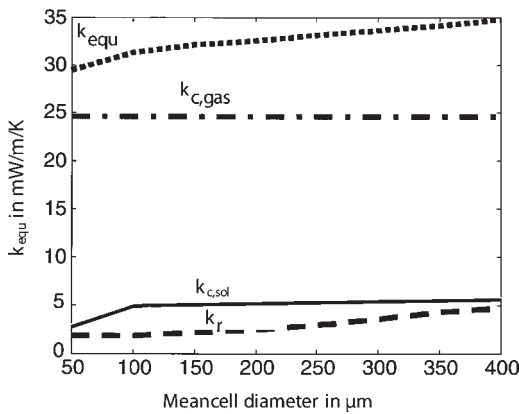


Figure 11.22 Equivalent thermal conductivity of PUR foams versus foam density (at 300 K, for 35 kg m^{-3} foam density and $3 \mu\text{m}$ strut diameter) [2].

Concerning the conductive properties, the effective phonic conductivity is obtained by the analytical model of Schuetz and Glicksman (Eq. (11.1)) with a proportion of solid in the struts $f_s = 1$ and a conductivity of metal $k_{\text{metal}} = 10 \text{ W m}^{-1} \text{ K}^{-1}$ which is a typical value for metals.

The computation of the equivalent thermal conductivities of metallic foams is carried out for different porosities, mean cell diameters, reflectivities and different parameters of specularity using a numerical resolution of the radiation–conduction coupling.

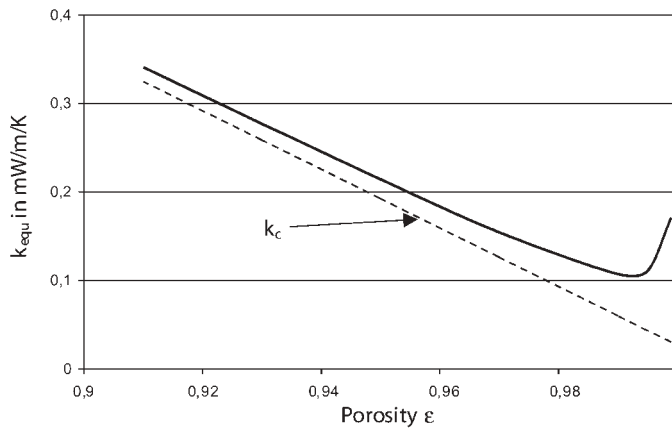


Figure 11.23 Evolution of the equivalent conductivity with the porosity.

Influence of the Porosity The variations of the equivalent thermal conductivity at ambient temperature ($T = 296$ K) with the porosity of the foam are illustrated in Figure 11.23 assuming a gray, specularly reflecting solid phase ($p_{sp\lambda} = 1.0$) with $\rho_\lambda = 0.9$ and a mean cell diameter $D_{cell} = 2.57$ mm.

The results of the model show that the equivalent conductivity of metallic foams reaches a minimum value for a porosity value. This variation of the thermal performances with the porosity is encountered in almost all porous materials in which there is a conflicting evolution of the conductive and radiative contributions with the porosity. In Figure 11.23, the evolution of the effective phonic conductivity k_c of the foam is also depicted and illustrates explicitly that, from a given optimal porosity, the decrease of k_c due to the increasing porosity is entirely balanced by an increase of the radiative heat transfer. However, in the case of metallic foams, one can notice that the optimum is obtained for a relatively high porosity (close to 0.99).

Influence of the Cell Diameter Figure 11.24 shows the evolution of the total conductivity of metallic foams with the diameter of the cells forming the porous structure for three different porosities commonly encountered ($\varepsilon = 0.98, 0.96$ and 0.94). As in the previous section, the solid phase is assumed gray and specularly reflecting ($p_{sp\lambda} = 1.0$ and $\rho_\lambda = 0.9$) and the calculations were carried at ambient temperature (296 K).

The results of the model assuming dodecahedral cells with no accumulation of matter at the junction of struts indicate that D_{cell} influences significantly the heat transfer in metallic foams. Indeed, whatever the porosity, foams with relatively small cells have better insulating performances. The results also reveal that the differences are entirely due to the radiative contribution given that, for a given porosity, the contribution of conductive heat transfer (k_c) does not vary with D_{cell} . Thus, small cells make the foam more opaque to thermal radiation. One can also remark that the theoretical increase of k_{equ} with the diameter of the cells is almost linear. Finally, we remark that, at ambient temperature and for the range of porosities considered,

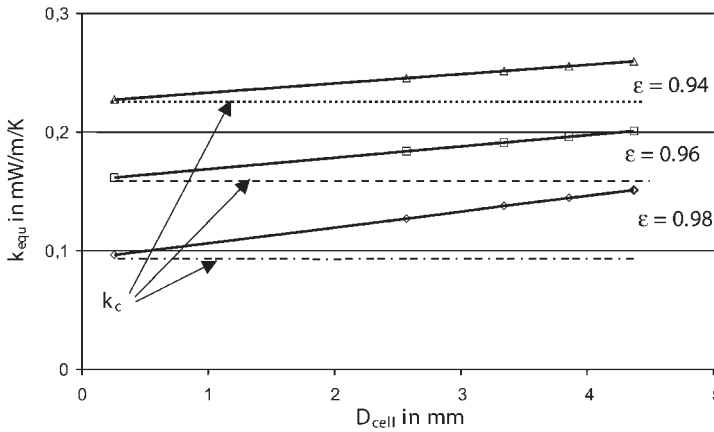


Figure 11.24 Evolution of the equivalent conductivity with the mean cell diameter for different porosities.

the radiative heat transfer is practically negligible as soon as the diameter of the cells is less than 1 mm.

Although we only illustrated the results obtained for dodecahedral cells composed of struts with constant triangular cross-sections, it is important to indicate that all the previous remarks are valid whatever the shape of the cells and of the struts.

Influence of the Reflectivity and Metal Specularity Parameter The other parameters which influence the thermal behavior of metallic foams are related to the reflecting properties of the solid phase. In real metallic foams, the proportion of thermal radiation reflected by the solid phase depend on numerous parameters including the nature of the metal considered, the surface roughness or the angle of incidence of the radiation on the solid/gas interface. Moreover, the radiant energy may be reflected specularly or diffusely. In order to simplify the problem and be able to investigate the influence of reflecting properties, we have seen that Loretz *et al.* [26] assumed that the reflectivity ρ_λ is independent of the incident angle and that the foam presents an intermediate reflecting behavior characterized by specularity parameter $p_{sp\lambda}$. The influence of the two parameters on the equivalent thermal conductivity is shown in Figure 11.25 for foams with $\varepsilon = 0.98$, $D_{cell} = 2.57$ mm at ambient temperature.

The results obtained using the hypothesis adopted by Loretz *et al.* show that the influence of the reflectivity of the solid phase depends on the way the radiation is reflected. Then, we note that when the reflection is specular, the reflectivity does not influence the radiative heat transfer. When $p_{sp\lambda}$ is close to 0, a high reflectivity results in a smaller equivalent conductivity. For example, the theoretical difference between a purely reflecting and a purely absorbing solid phase reaches $10 \text{ mW m}^{-1} \text{ K}^{-1}$ when the reflection is assumed diffuse ($p_{sp\lambda} = 0.0$) which represent more than 8% of the total conductivity and 38% of the radiative contribution. This can be explained by the fact that the scattering phase function of the foam is, then, $P(\theta) = (8/3\pi)(\sin\theta - \theta\cos\theta)$

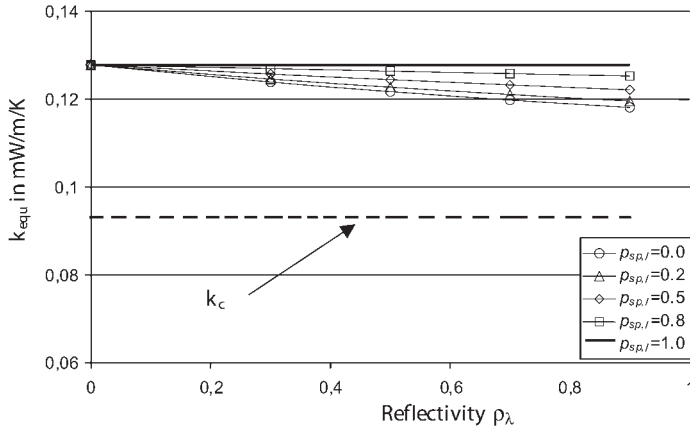


Figure 11.25 Evolution of the equivalent conductivity with the reflectivity for different parameters of specularity.

and most of the radiant energy reflected is reoriented in backward directions which slows down the radiative heat flux. When the reflection is specular ($p_{sp,\lambda} \rightarrow 1$), the phase function is isotropic and, thus, the radiant energy reflected is redistributed in all directions with the same probability as if it has been absorbed and reemitted by the solid phase.

11.6.3.4 Open-Cell Carbon Foams

The influence of the temperature on the foam equivalent conductivity is also very important. To illustrate this phenomenon we choose to show some results obtained by Baillis *et al.* [39] for carbon foams. Such materials can be used as insulating media at very high temperature.

The gas is nitrogen. Its conductivity is defined by the following relation:

$$k_{\text{gas}} = k_0 \left(1 + \frac{C}{273} \right) \frac{\sqrt{T/273}}{1 + (C/T)} \quad (11.45)$$

where $k_0 = 0.0242 \text{ W m}^{-1} \text{ K}^{-1}$ and $C = 161 \text{ K}$. T is in kelvin.

Experimental results of equivalent total conductivity obtained from guarded hot-plate measurements are compared with theoretical results obtained using the experimental value of carbon conductivity, $k_{\text{carbon}} = 22 \text{ W m}^{-1} \text{ K}^{-1}$. The effective phonic conductivity is deduced from the analytical model of Schuetz and Glicksman (Eq. (11.1)) and the radiative properties are obtained from the predictive model already described in Section 11.5.3.1. The foam porosity is 98.75%. The sample thickness is 10 mm. Experimental and theoretical total conductivities and the phonic effective conductivity are shown in Figure 11.26 as a function of the hot face temperature. It can be observed that at high temperatures, radiative transfer is preponderant. Moreover, experimental and theoretical conductivities are in good agreement; these results confirm that the predictive model is appropriate to

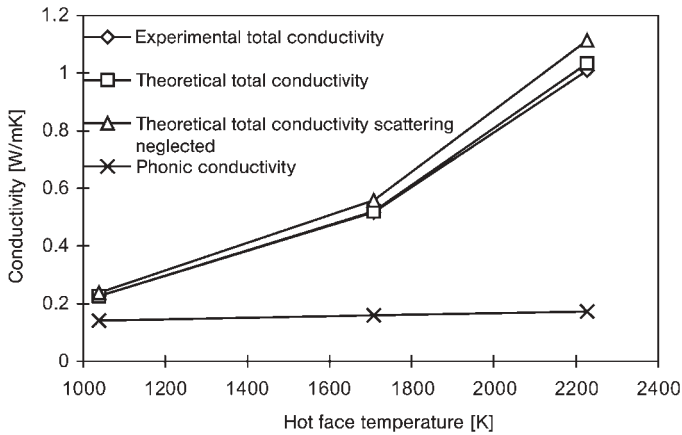


Figure 11.26 Equivalent conductivity of carbon foam sample [39].

determine the thermal properties. Note that for carbon foam since the carbon reflectivity is not very high in the visible range, there is not a great deviation if scattering phenomena are neglected.

11.7 Conclusions

Thermal properties of usual cellular foam such as carbon or metallic open-cell foams or EPS, XPS and PUR closed-cell foams have been investigated. It appears that in such foams the radiative transfer contributes significantly to the total heat transfer and that it is preponderant at high temperatures. Moreover, we pointed out that the geometrical structure of the cellular material greatly affects their thermal properties. Thus, theoretical models are very useful to investigate the influence of the parameters characterizing the microstructure on the foam equivalent thermal conductivity and to optimize foam thermal performances. The equivalent conductivity could be improved by modifying wall thickness, strut diameters, cell diameters or foam densities. The theoretical results show that the density and the mean cell diameter are generally the most sensitive parameters. Moreover, the cells forming the cellular materials could be tetrakaidecahedrons, cubes or dodecahedrons. The analysis of the results for these three different cell shapes also indicates a non-negligible influence on the thermal behavior of the foam.

The first works which tried to predict the heat transfer in such complex materials used drastic simplifications, and some noticeable improvements have been achieved in the field recently. New models designed to predict conductive and radiative coupled heat transfer in low-density foams have been proposed recently. The radiation-conduction coupling is solved using accurate numerical methods for the resolution of the energy equation and the radiative transfer equation. The models developed to predict the conductive and radiative properties try to take into

account more faithfully the real morphologies of foam. Moreover, predictive models of radiative properties take into account more and more precisely the scattering behavior of solid matter.

However, the usual analyses in the literature generally assume that the foams are homogeneous and isotropic. Moreover, the cell and strut diameters are usually assumed constant and dependent scattering is generally neglected. All these assumptions should be verified in the future.

Moreover, the determination of foam radiative properties at temperatures higher than room temperature remains an open problem. Actually, it is difficult to find in the literature experimental data on the thermal properties of carbon or metallic foams for the temperature range of interest. Thus, the extension of the classical methods, enabling the experimental characterization of radiation and conduction properties of foams to higher temperatures, seems to be one of the challenging prospects of research in the field as it presents much interest for numerous technological applications.

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12

On the Application of Optimization Techniques to Heat Transfer in Cellular Materials

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and Miguel Vaz Junior*

12.1

Introduction

A steady increase has been observed in recent years in the use of cellular materials based on several different topologies. Applications range from mechanical energy absorbers to filters, pneumatic silencers/sound absorbers, containment matrices and burn rate enhancers for solid propellants, flow straighteners, catalytic surfaces for chemical reactions, core structures for high strength panels, heat sinks and heat exchangers in general [1,2]. Furthermore, from a combined structural and thermal viewpoint, cellular materials have also been proposed as viable alternatives for high-impact and low-weight applications, such as actively cooled structural elements for satellites or hypersonic aircraft wings [3]. Recent advancements in manufacturing processes have made possible a realization of such applications, instigating further studies on the improvement of the structural and thermal efficiency of both open and closed cell structures.

The literature shows intense and healthy discussions on the recommended cell topology for a given application. In general, cellular structures can be categorized as (a) open or closed cellular materials and (b) stochastic or regular cellular structures [4]. Researchers tend to acknowledge that stochastic metal foams with open cells have better thermal, acoustic and energy absorption properties; however, their load-bearing capability is significantly inferior to periodic structures with the same weight [5]. Within the framework of heat transfer applications, Lu and Chen [6], by advocating open-celled foams, emphasize that transport properties of cellular materials are of considerable practical interest in fields such as thermal insulation, reservoir engineering and underground storage of nuclear wastes. In addition, the authors remark that applications which demand high efficiency in heat dissipation, such as heat sinks for high-power electronic devices operating at power densities in excess of 10^7 W m^{-2} , make open-celled metallic foams very attractive heat exchangers. Zhao *et al.* [2] point out that open-cell metal foams are also regarded as one of

the most promising materials for manufacturing heat exchangers due to the high surface area density and strong mixing capability for the fluid. On the other hand, Seepersad *et al.* [3] ponder that prismatic/periodical cellular materials, or purpose-tailored extruded metal honeycombs, are well-suited for ultralight structures, fuel cell and battery subsystems, and energy absorption systems.

Further enhancement of both heat transfer and structural/topological characteristics can be achieved by application of optimization strategies to the geometrical parameters of cellular materials.

The optimum design can be determined by using basically three distinct approaches: size, shape and topology optimization. The first strategy aims at determining the optimum design by optimizing one or more global characteristic parameters of a cellular structure, while preserving its generalized shape. Shape optimization consists of finding the overall boundary shape of a structure made of a cellular material, such that the *structure* is able to reach an optimum thermal performance. Alternatively, a problem can be proposed to find the shape of inclusions/voids in a periodic cell, such that the *material* is able to reach an optimum thermal performance. A more general procedure is provided by topology optimization, which allows insertion of new porous surfaces and local variations of geometrical characteristics of the cellular materials. Again, the objective might be to optimize a structure or the material itself. A detailed presentation of the material optimization case – or material design – is the subject of Section 12.3.

This chapter addresses application of some of the previous optimization strategies to both metal foams and regular cell structures. Section 12.2 discusses optimization issues, including generalities on evolutionary methods and gradient based mathematical programming. Section 12.3 introduces the concept of periodic composite materials and presents theoretical and numerical aspects related to homogenization and optimization of unit cells, extensive to functionally graded materials. Section 12.4 presents a general overview of recent works on optimization of cellular-type materials, and Section 12.5 introduces original results of optimized microstructures using the topology optimization/functionally graded materials approach proposed in Section 12.3. Finally, some concluding remarks are presented in Section 12.6.

12.2 Optimization Approaches

Size, shape and topology optimization strategies have been used by researchers to tailor the microstructure of cellular materials to fit specific needs. In this chapter, we review some of these applications and propose a strategy which employs *functionally graded materials* to optimize heat conduction properties. In this regard, the present section briefly sets the general optimization problem to be solved in material or structural design and presents some concepts related to the optimization strategies described in the literature. Basically, evolutionary methods and gradient-based mathematical programming approaches are considered.

The typical optimization problem to be solved is of the type:

$$\begin{aligned}
 &\text{Minimize} && g_0(\mathbf{b}) && \mathbf{b} \in \mathbf{R}^n \\
 &\text{Subject to} && h_i(\mathbf{b}) = 0 && i = 1 \dots l \\
 &&& g_j(\mathbf{b}) \leq 0 && j = 1 \dots m \\
 &&& \underline{b}_k \leq b_k \leq \bar{b}_k && k = 1 \dots n
 \end{aligned} \tag{12.1}$$

where $\mathbf{b} \in \mathbf{R}^n$ is a vector of *design variables* which is limited by upper and lower bounds $\bar{b}_k$ and $\underline{b}_k$, $g_0(\mathbf{b})$ is the *objective function* to be minimized and $h_i(\mathbf{b})$ and $g_j(\mathbf{b})$ are equality and inequality constraints respectively. The functions generally depend nonlinearly on the design variable vector $\mathbf{b}$, and the dependence can be either implicit or explicit. Gradient-based solution procedures additionally require continuity and twice differentiability in $\mathbf{R}^n$. The region of $\mathbf{R}^n$ over which all the constraints are satisfied is named the *feasible region*.

12.2.1

Evolutionary Algorithms (EAs)

An EA is a generic population-based optimization algorithm that uses concepts and mechanisms inspired in biological evolution. The common underlying idea behind all EA variants is that each candidate solution plays the role of an individual taken from a population, and that some individuals in each population are selected to generate next generations. Selection and evolution of the population takes place after recursive application of some operators that mimic biological evolution, as for instance, combination and mutation.

These kinds of algorithm require neither derivative information nor further knowledge about the functions involved, making them prone to deal with discontinuous and/or non-convex problems. Additionally, their intrinsic parallel nature and their possibility to provide a number of potential solutions to a given problem, make them well-suited to solve multiobjective optimization and scheduling problems [7]. EAs have been successfully applied to the optimization of heat properties of cellular and porous materials [8–10]. Most solutions have been proposed for microchannel heat sinks aiming at improving the cooling capacity of electronic components [8,9]. In such problems, the design variables for the EAs are, in general, the aspect ratio and wall thickness of the channel cell and the channel length and width, with constraints such as pumping power and pressure drop. Individual solutions can define additional design variables and constraints. Further details on the solution strategies are presented in Section 12.4.

12.2.1.1 Basic Concepts in Evolutionary Algorithms

In the realm of EAs, different variations can be found in the literature. Some examples are genetic algorithms, evolutionary programming, evolution strategy, genetic programming, differential evolution, particle swarm optimization, and so forth. An EA can be described by some basic concepts, which must be defined in order to properly characterize a particular approach [11]. These concepts include the

representation of an individual, population, fitness or evaluation function, parent selection mechanism, variation operators and survivor selection mechanism (replacement). Each of these basic components is briefly presented in the following paragraphs.

- Representation of an individual. Each individual is represented by a set of design variables, usually in vector form. As EAs mimic nature when seeking potential solutions for a given problem, this vector is called a *chromosome* and each design variable is called a *gene*. Each gene can be represented in many ways such as binary strings, floating point numbers, gray encoding, and so forth.
- Population. One of the main differences of EAs when compared to traditional approaches is the use of many individuals in each iteration. The set containing the potential solutions or individuals in each iteration is called a *population* and the form in which each iteration is related to a particular evolving population is called a *generation*. The population size can be changed in each generation.
- Fitness function. The fitness is a mapping between a set containing the design variables associated with an individual (chromosome) and a real value. This real value is used as a measure of quality of the corresponding individual. The fitness can be the value of an objective function, some linear combination of the objective function and constraints, and so forth.
- Parent selection mechanism. At each generation, a new population is formed by the combination of the chromosomes of some individuals of the previous population. It is necessary to establish a criterion, known as *parent selection mechanism* or *mate selection*, to choose the individuals to combine. This criterion selects a set of individuals in the population, which are combined to generate a new population. There are many criteria in the literature and diversity is one of the main issues in this selection, since the combination of only the *best* individuals in each population would lead to local minima.
- Variation operators. The objective of a variation operator can be either to modify the chromosome of some individuals of the population or to recombine the chromosomes of some pre-selected individuals of the population. The modification of the chromosome of some individuals can be achieved by heuristic rules or by *mutation*, which is a random change in some parts of the chromosome. The recombination of individuals to form new ones is achieved by mixing two individuals with different (but desirable) chromosomes. This procedure can be regarded as a search in the design space and is one of the most important features of EAs. Both, modification and recombination are strongly related to the representation of an individual. Thus, the operators used in a binary representation are different from the operators used in a floating-point representation.
- Survival mechanism. Survival mechanism or replacement is the operation used to select which individuals of the new population will overwrite the individuals of the

previous population. This mechanism can be seen as an environmental selection and is usually deterministic.

12.2.2

Mathematical Programming using Gradient-Based Procedures

While shape optimization typically deals with few design variables which define the shape of a component, a structure or simply a region in space, topology optimization deals with material distribution and the design variables are local densities defined at each node or element. Thus, in this case, the optimization problem may easily involve thousands of design variables. Hence, algorithms well adapted for shape optimization will not necessarily be efficient for topology optimization. In practice, there is a general preference of *sequential quadratic programming* (SQP) for shape optimization [12] whereas *sequential linear programming* (SLP) and separable *sequential convex programming* (SCP) – including CONLIN and the MMA family algorithms – are preferred for topology optimization applications [13,14]. The literature shows that most solutions associated with optimizing thermal characteristics of cellular structures approach the problem using topology optimization (see Refs [15,16] and references therein). For instance, under the total material volume constraint, both relative density and cell size distribution can be optimized either to enhance insulation under radiation heat transfer or to improve cooling capacity in electronic components. Shape optimization can also be used to design either void/inclusion shapes of periodical cells or the cellular structure aiming at enhancing thermal performance. Section 12.3 presents applications of gradient based shape and topology optimization for designing periodic cellular materials with enhanced thermal properties.

12.3

Periodic Composite Materials

A special class of cellular material is the one which has regular periodicity, meaning that its mechanical, thermal or any other physical characteristics have the following property [17]:

$$\mathcal{F}(\mathbf{x} + \mathcal{N}\mathbf{Y}) = \mathcal{F}(\mathbf{x}) \quad (12.2)$$

where $\mathcal{F}$ is the property, $\mathbf{x} = [x_1, x_2, x_3]^T$ is the position vector of a point, $\mathcal{N}$ is a 3×3 diagonal matrix

$$\mathcal{N} = \begin{bmatrix} n_1 & 0 & 0 \\ 0 & n_2 & 0 \\ 0 & 0 & n_3 \end{bmatrix} \quad (12.3)$$

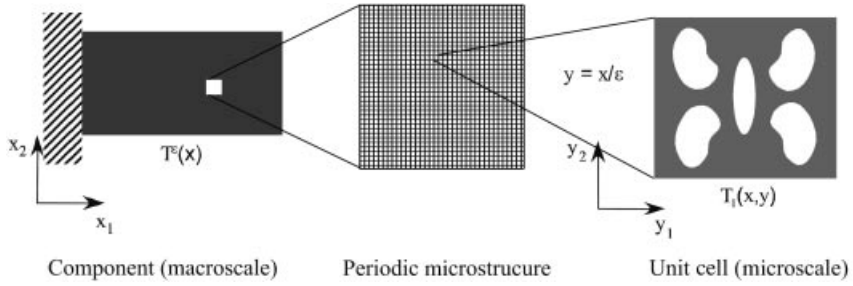


Figure 12.1 Concept of multiscale showing the macro-dimensions ($\mathbf{x}$) and micro-dimensions ($\mathbf{y}$) in two-dimensions.

in which n_1 , n_2 and n_3 are arbitrary integer numbers and $\mathbf{Y}=[Y_1, Y_2, Y_3]^T$ is a constant vector which determines the period (unit cell dimension) of the structure. The period is usually assumed to be very small compared to the dimension of the overall domain, and thus the mechanical, thermal or physical characteristics of the medium experience rapid oscillations in the neighborhood of a point $\mathbf{x}$.

Figure 12.1 depicts a two-dimensional (2D) example of a periodic composite in which rapid oscillations are expected in the temperature field. In the figure, ε is a parameter of small magnitude representing the microscale in which the properties are changing (composite microstructure scale), and $\mathbf{x}$ and $\mathbf{y}$ are the coordinates associated with the composite macro- and micro-dimensions, respectively.

12.3.1

Homogenization of Heat Properties in Periodic Composite Materials

Homogenization allows the calculation of the effective properties of a complex periodic composite material from its unit cell topology (see Figure 12.1). It is a general method for calculating effective properties and has no limitations regarding volume fraction or shape of the composite constituents. The main assumptions are that the unit cell is periodic and that the scale of the composite part is much larger than the microstructure dimensions [18].

This section addresses details of the theoretical and computational aspects of the homogenization method applied to composites for heat transfer applications. Considering the standard homogenization procedure for heat conduction materials, the unit cell is defined as $\mathbf{Y}=[0, Y_1] \times [0, Y_2] \times [0, Y_3]$ and the thermal conductivity property function k_{ij} is considered to be a $\mathbf{Y}$ -periodic function:

$$\mathbf{k}^\varepsilon(\mathbf{x}) = \mathbf{k}(\mathbf{x}, \mathbf{y}); \quad \mathbf{k}(\mathbf{x}, \mathbf{y}) = \mathbf{k}(\mathbf{x}, \mathbf{y} + \mathbf{Y}) \quad \text{and} \quad \mathbf{y} = \mathbf{x}/\varepsilon, \varepsilon > 0 \quad (12.4)$$

where ε is the length-scale parameter, and $\mathbf{x}$ and $\mathbf{y}$ are the coordinates associated with the composite macro- and micro-dimensions, according to Figure 12.1. Expanding

the temperature T inside the unit cell [18], one gets

$$T^\varepsilon = T_0(\mathbf{x}) + \varepsilon T_1(\mathbf{x}, \mathbf{y}) \quad (12.5)$$

in which a single-length-scale approach is adopted, that is, only the first-order variation terms $T_1(\mathbf{x}, \mathbf{y})$ are accounted for, and T_1 is $\mathbf{Y}$ -periodic.

The temperature gradient is written as [18,19]

$$\nabla_x T^\varepsilon = \nabla_x T_0(\mathbf{x}) + \varepsilon \nabla_x T_1(\mathbf{x}, \mathbf{y}) + \nabla_y T_1(\mathbf{x}, \mathbf{y}) \quad (12.6)$$

and, by definition

$$(\nabla_x)_i(\cdot) = \frac{\partial(\cdot)}{\partial x_i}; \quad (\nabla_y)_i(\cdot) = \frac{\partial(\cdot)}{\partial y_i} \quad (12.7)$$

Equations (12.5) and (12.6), together with properties (12.4) are replaced into the energy functional for the thermal conductivity medium, given by

$$G(T^\varepsilon) = -\frac{1}{2} \int_{\Omega} [\nabla_x T^\varepsilon]^T \mathbf{k}^\varepsilon \nabla_x T^\varepsilon d\Omega + \int_{\Gamma} q T^\varepsilon d\Gamma \quad (12.8)$$

where q is the surface heat flux, which is assumed independent of the microstructure scale ε , and Ω and Γ are the domain and boundary of the macroscopic composite structure, respectively. After substituting Eqs. (12.4), (12.5) and (12.6) into (12.8), one obtains

$$\begin{aligned} G(T^\varepsilon) = & -\frac{1}{2} \int_{\Omega} [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})] d\Omega \\ & - \varepsilon \int_{\Omega} [\nabla_x T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})] d\Omega \\ & - \frac{\varepsilon^2}{2} \int_{\Omega} [\nabla_x T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_x T_1(\mathbf{x}, \mathbf{y}) d\Omega \\ & + \int_{\Gamma} q T_0(\mathbf{x}) d\Gamma + \varepsilon \int_{\Gamma} q T_1(\mathbf{x}, \mathbf{y}) d\Gamma \end{aligned} \quad (12.9)$$

Taking the G -differential of $G(T^\varepsilon)$ at T^ε and passing to the limit $\varepsilon \rightarrow 0$ in $G(T^\varepsilon)$:

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \{\delta G(T^\varepsilon)\} = & - \int_{\Omega} [\nabla_x \delta T_0(\mathbf{x}) + \nabla_y \delta T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \\ & [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})] d\Omega + \int_{\Gamma} q \delta T_0(\mathbf{x}) d\Gamma = 0 \end{aligned} \quad (12.10)$$

for every admissible $\delta T_0(\mathbf{x})$ and $\delta T_1(\mathbf{x}, \mathbf{y})$. Now, using that [18]

$$\lim_{\varepsilon \rightarrow 0} \int_{\Omega} \Phi\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) d\Omega = \lim_{\varepsilon \rightarrow 0} \frac{1}{|Y|} \int_{\Omega} \int_Y \Phi\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) dY d\Omega \quad (12.11)$$

where Φ denotes the function of interest and Y is the unit cell (microscopic) domain, the following relation must hold to satisfy Eq. (12.10):

$$-\int_{\Omega} \frac{1}{|Y|} \int_Y [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_x \delta T_0(\mathbf{x}) dY d\Omega + \int_{\Gamma} q \delta T_0(\mathbf{x}) d\Gamma = 0 \quad (12.12)$$

for every admissible $\delta T_0(\mathbf{x})$, and

$$-\int_{\Omega} \frac{1}{|Y|} \int_Y [\nabla_x T_0(\mathbf{x}) + \nabla_y T_1(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_x \delta T_1(\mathbf{x}, \mathbf{y}) dY d\Omega = 0 \quad (12.13)$$

for every admissible $\delta T_1(\mathbf{x}, \mathbf{y})$.

Equations (12.12) and (12.13) are called macroscopic and microscopic equations, since they contain terms related to $\delta T_0(\mathbf{x})$ and $\delta T_1(\mathbf{x}, \mathbf{y})$, respectively. Due to the linearity of the problem, and by assuming the separation of variables for $T_1(\mathbf{x}, \mathbf{y})$, one gets

$$T_1(\mathbf{x}, \mathbf{y}) = R^{(m)}(\mathbf{x}, \mathbf{y}) \frac{\partial T_0}{\partial x_m} \Rightarrow \nabla_y T_1(\mathbf{x}, \mathbf{y}) = \nabla_y \mathbf{R}(\mathbf{x}, \mathbf{y}) \nabla_x T_0(\mathbf{x}) \quad (12.14)$$

where $R^{(m)}(\mathbf{x}, \mathbf{y})$ are the characteristic temperatures of the unit cell due to each possible initial temperature gradient, which is also Y -periodic, belonging to $H_{\text{per}}(Y)$: $H_{\text{per}}(Y) = \{v \in H^1(Y) \mid v \text{ takes equal values on opposite sides of } Y\}$, which corresponds to the periodicity condition in the unit cell (see Figure 12.2). $\mathbf{R}$ is a line matrix given by $[R^{(1)} R^{(2)}]$ in 2D and $[R^{(1)} R^{(2)} R^{(3)}]$ in 3D.

Therefore, replacing Eq. (12.14) into the microscopic Eq. (12.13), we obtain [18,19]

$$-\int_{\Omega} \frac{1}{|Y|} \int_Y [\nabla_x T_0(\mathbf{x}) + \nabla_y \mathbf{R}(\mathbf{x}, \mathbf{y}) \nabla_x T_0(\mathbf{x})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_x \delta T_1(\mathbf{x}, \mathbf{y}) dY d\Omega = 0 \quad (12.15)$$

$\forall \delta T_1 \in H_{\text{per}}(Y)$

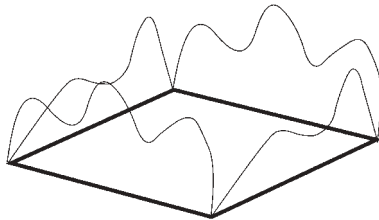


Figure 12.2 Periodicity conditions in the unit cell.

This equation can be satisfied if $\mathbf{R}(\mathbf{x}, \mathbf{y})$ is the solution of

$$\frac{1}{|Y|} \int_Y [I + \nabla_{\mathbf{y}} \mathbf{R}(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{y}} \delta T_1(\mathbf{x}, \mathbf{y}) dY = 0 \quad \forall \delta T_1 \in H_{\text{per}}(Y) \quad (12.16)$$

which can be rewritten using the index notation:

$$\frac{1}{|Y|} \int_Y k_{ij}(\mathbf{x}, \mathbf{y}) \left(\delta_{im} + \frac{\partial R^{(m)}}{\partial y_i} \right) \frac{\partial (\delta T_1)}{\partial y_j} dY = 0 \quad \forall \delta T_1 \in H_{\text{per}}(Y) \quad (12.17)$$

Substituting Eq. (12.14) into the macroscopic Eq. (12.12), we obtain

$$\begin{aligned} & - \int_{\Omega} \frac{1}{|Y|} \int_Y [\nabla_x T_0(\mathbf{x}) + \nabla_{\mathbf{y}} \mathbf{R}(\mathbf{x}, \mathbf{y}) \nabla_x T_0(\mathbf{x})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) \nabla_x \delta T_0(\mathbf{x}) dY d\Omega \\ & + \int_{\Gamma} q \delta T_0(\mathbf{x}) d\Gamma = 0 \end{aligned} \quad (12.18)$$

Thus, the definition of the effective properties is obtained [18]:

$$\mathbf{k}^H = \frac{1}{|Y|} \int_Y \mathbf{k}(\mathbf{x}, \mathbf{y}) [I + \nabla_{\mathbf{y}} \mathbf{R}(\mathbf{x}, \mathbf{y})] dY \quad (12.19)$$

and Eq. (12.18) can be written as

$$- \int_{\Omega} \nabla_x T_0(\mathbf{x}) \mathbf{k}^H \nabla_x \delta T_0(\mathbf{x}) d\Omega + \int_{\Gamma} q \delta T_0(\mathbf{x}) d\Gamma = 0 \quad (12.20)$$

for every admissible $\delta T_0(\mathbf{x})$. By using Eq. (12.16), one can easily show that Eq. (12.19) can be also written in the form

$$\mathbf{k}^H = \frac{1}{|Y|} \int_Y [I + \nabla_{\mathbf{y}} \mathbf{R}(\mathbf{x}, \mathbf{y})]^T \mathbf{k}(\mathbf{x}, \mathbf{y}) [I + \nabla_{\mathbf{y}} \mathbf{R}(\mathbf{x}, \mathbf{y})] dY \quad (12.21)$$

or using the index notation

$$k_{pq}^H(\mathbf{x}) = \frac{1}{|Y|} \int_Y k_{ij}(\mathbf{x}, \mathbf{y}) \left(\delta_{ip} + \frac{\partial R^{(p)}}{\partial y_i} \right) \left(\delta_{jq} + \frac{\partial R^{(q)}}{\partial y_j} \right) dY \quad (12.22)$$

and $k_{ij}^H = k_{ji}^H$.

The calculation of the effective properties can become computationally efficient by taking advantage of symmetry boundary conditions. An isotropic unit cell has symmetry relative to all axes; and an orthotropic unit cell has symmetry relative to both axes or only one axis. In this case, we can take advantage of these

properties to reduce the computational cost and to perform the optimization and homogenization in only one part of the domain. However, the appropriate boundary conditions must be considered for the displacement characteristic function $\mathbf{R}$ [18].

12.3.2

Functionally Graded Materials

Functionally graded materials (FGMs) possess continuously graded properties and are characterized by spatially varying microstructures created by nonuniform distributions of the reinforcement phase as well as by interchanging the role of reinforcement and matrix (base) materials in a continuous manner (see Figure 12.3). The smooth variation of properties may offer advantages such as reduction of stress concentration and increased bonding strength [20,21].

Standard composite materials result from the combination of two or more materials, usually resulting in materials that offer advantages over conventional materials. However, in traditional composites (e.g. laminated) there is a sharp interface among the constituent phases which may cause problems such as stress concentration, delamination and scattering (if a wave is propagating inside the material), among others. However, a material made using the FGM concept would maintain the advantages of traditional composites and eliminate problems related to the presence of sharp interfaces.

The continuous transition of FGM microstructure causes a nonuniform macroscopic distribution of properties, and thus the classic approach of calculating effective properties of composite material, which considers only the local characteristics of a *representative volume fraction* (RVE), may be limited [22]. Essentially, the hypothesis that the RVE dimensions are small enough in relation to, for example, the heat flux field variation in heat transfer problems may not be verified, once the macroscopic heat flux field may not be constant inside the RVE because the property

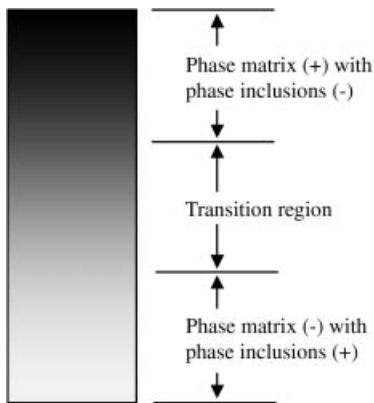


Figure 12.3 Schematic representation of microstructure change in an FGM.

gradation generates a heat flux field variation. In the context of elasticity, Pindera *et al.* [22] proposed a nonlocal high-order material model based on the *method of cells* [23], in which the properties at a point are dependent not only on the microstructure at that point but also on its gradation. Thus, the RVE concept is revised and this model can represent not only a structural point but an entire region and its gradation. Thus, the macrostress analysis is coupled to the microstress analysis. Another approach to calculate effective properties of FGMs was proposed by Yin *et al.* [24] and it is based on the extension of the Mori–Tanaka model in the sense that it considers the interaction among particles (inclusions in the matrix). In this approach, the RVE presents a heterogeneous material distribution which considers a gradient of inclusion distribution. However, methods to calculate FGM (and heterogeneous materials in general) effective properties by using nonlocal or high-order models are still an open problem in the literature [25,26].

Regarding the capacity of the traditional micromechanical models to calculate FGM effective properties, Reiter *et al.* [27] presented an interesting study about using Mori–Tanaka and self-consistent models to estimate these properties. The main conclusion is that these models can be applied to the regions where inclusion and matrix phases can be easily distinguished. For the transition region, these models will be valid depending on the ratio of phase properties.

Within the framework of designing cellular materials with the objective of improving thermal characteristics, the FGM concept can be employed in two basic ways. In the first one, material gradation is optimized over the whole structure, so that an optimum distribution of the void fraction is determined. This strategy was used, for instance, by Zhu *et al.* [28] to design metallic foams aiming at enhancing thermal insulation. Alternatively, FGMs can be applied using a periodical cell strategy. In this case, material gradation is defined within a unit cell using periodic boundary conditions. The mathematical and numerical formulation introduced in this section and the results discussed in Section 12.5 are focused on the latter approach.

12.3.3

Numerical Implementation of Homogenization

The numerical implementation of homogenization is presented considering the continuous approximation of material distribution (CAMD) concept [29]. Equation (12.16) is solved using the finite element method (FEM). The unit cell is discretized by N finite elements:

$$Y = \cup_{e=1}^N \Omega^e \quad (12.23)$$

where Ω^e is the domain of each element. Thus, the characteristic functions previously defined are expressed in each element as a function of the shape functions (N_I):

$$R^{(p)} \cong \sum_{I=1}^{n_d} N_I R_I^{(p)} \quad (12.24)$$

Similar relations hold for δT_1 . Substituting Eq. (12.24) in Eq. (12.16), and assembling the individual matrices for each element, we obtain the following global matrix system for each load case p :

$$\mathbf{C}\hat{\mathbf{R}}^{(p)} = \mathbf{Q}^{(p)} \quad (12.25)$$

where $\hat{\mathbf{R}}^{(p)}$ is a vector containing the corresponding nodal values of the characteristic function $\mathbf{R}^{(p)}$, respectively. The global conductivity matrix is the assembly of each element's individual matrix, and the global heat flux vector ($\mathbf{Q}^{(p)}$) is the assembly of the individual heat flux vectors for all elements:

$$\mathbf{C} = \mathbf{A}_{e=1}^N \mathbf{C}^e; \quad \mathbf{Q}^{(p)} = \mathbf{A}_{e=1}^N \mathbf{Q}^{e(p)} \quad (12.26)$$

where $\mathbf{A}$ is the assembly operator. The element matrices and vectors are given by the expressions

$$\mathbf{C}_{IJ}^e = \int_{\Omega^e} k_{ij}^e \frac{\partial N_I}{\partial y_i} \frac{\partial N_J}{\partial y_j} d\Omega^e; \quad \mathbf{Q}_I^{e(p)} = \int_{\Omega^e} k_{jp}^e \frac{\partial N_I}{\partial y_j} d\Omega^e \quad (12.27)$$

Thus, for the 2D problem, there are two load cases to be solved independently. They come from Eq. (12.25), where the index p can be 1 or 2. All load cases must be solved by enforcing periodic boundary conditions in the unit cell for the temperature (see Figure 12.2).

In addition, when the unit cell is made of an FGM material, the material properties change gradually inside of the element domain, and thus the material property must be kept inside of the integral during numerical integration, using the graded finite element concept [30] (see Figure 12.4).

Regarding the numerical solution of the matrix system given by Eq. (12.26), the total matrix bandwidth is spoiled due to the enforcement of the periodicity conditions. This increases the amount of memory storage necessary for the matrix. This problem can be avoided when the unit cell is symmetric. In this case, we consider the symmetry boundary conditions [18], instead of the periodicity conditions.

The temperature of some point of the unit cell must be prescribed to overcome the non-unique solution of the problem; otherwise the FEM problem will be ill-posed.

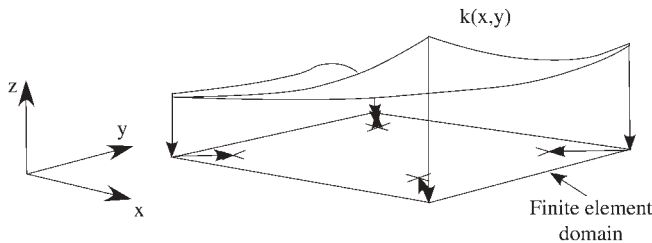


Figure 12.4 Continuous material distribution using graded finite element (material properties are evaluated at Gauss points).

The choice of this point with prescribed values does not affect the homogenized coefficients since only the derivatives of the characteristic functions are used in their computation.

12.3.4

Material Design: Shape and Topology Optimization of a Unit Cell

The unit cell is the smallest structure that is periodic in the composite matrix (see Figure 12.1). By changing the volume fraction of the constituents, the shape of the voids/inclusions, or even the topology of the unit cell, different effective properties for the composite material can be obtained. Therefore, when designing composites the properties to a specific application can be tailored, this cannot be done with a single material. The design of the composite material itself is a difficult task, and the design of a composite where the properties of its constituent materials change gradually in the unit cell domain is even more complex. Meanwhile, this design can be successfully achieved by using a *material design method*.

The overall objective of material design is to generate composites with prescribed or improved properties not found in common materials. This can be achieved by modifying the microstructure of the composite material. In traditional composite designs, such as fiber- or sphere-reinforced and laminated materials, the change in the properties is obtained by modifying the location, orientation, material constituents or volume fraction of the fiber, sphere or laminar inclusion. This allows some control of the composite properties. A more systematic approach to design composite materials has been developed in recent years, which combines shape/topology optimization with homogenization to change the composite material unit cell shape/topology until desired properties or performance are obtained for the composite. The approach consists of finding the shape and/or distribution of the material and void phases in a periodic unit cell that optimizes the properties or performance characteristics of the composite system. It is relevant to mention that, in this discussion, the general term *composite materials* encompasses cellular structures within the principle that a void is a special type of inclusion.

In the last few years, the material design concept based on topology optimization and homogenization has been applied to design elastic [31–33], thermoelastic and thermal conductivity [34–37], piezoelectric [38,39], phononic and photonic bandgap materials [40,41], among others. Shape optimization and homogenization has been applied by various researchers [12,42–45].

Torquato *et al.* [37] present an interesting discussion about designing of composites with multifunctional characteristics considering simultaneously thermal and electrical conductivity properties. Manufacturing techniques have also been studied to build such materials [46–49]; however, processing techniques have not been much explored when material gradation is considered inside the unit cell, rather than the traditional (1–0) design [49].

In the process of designing materials with prescribed and improved properties, a natural question related to the achievable properties in the material design process

arises. Based on the fact that the constitutive elasticity matrix must be positive definite for elastic materials, Milton and Cherkaev [50] show the existence of materials for all thermodynamically admissible sets by layering and combining an infinitely rigid material with voids (infinite compliant). However, the extreme condition of this admissible set, such as isotropic material with Poisson's ratio equal to -1 ($\nu = -1$), cannot be reached in practice since an infinitely rigid material does not exist.

Other bounds were derived in the past. Considering materials with finite properties, for example, Hashin and Shtrikman [51] proposed elastic and conductivity property bounds for an isotropic mixture of classical materials using energy analyses. Lipton and Noethrup [52] (among others) defines also bounds for orthotropic mixtures of isotropic materials. Bounds for elastic and conductivity properties of mixtures of two materials (not necessarily isotropic) were developed by Gibiansky and Torquato [53]. However, the extremal properties that can be achievable by composite designs is limited, and has been explored mainly for elasticity and conductivity [54,55].

12.3.4.1 Shape Optimization

The application of shape optimization for optimizing properties of a cellular material starts by the parameterization of the boundary of the void or inclusion. A possible approach is to work on the geometrical model using splines to define the boundary curve. In this case, the design variables can be the spline's control points or its knots. Since the mesh is attached to the boundary, when the spline suffers a perturbation, the mesh follows. This dependence is given by the so-called *velocity field*. Another possibility is to work on the discretized model by adopting directly nodal coordinates as design variables. Although this option has several well-known drawbacks [56], its use in this kind of application is frequent [12,43,44].

Figure 12.5 depicts a periodic cell with an inclusion shape parameterized by a curve, whose control points are allowed to move in the direction normal to the boundary. To solve this problem, periodic boundary conditions are imposed and the numerical homogenization procedure detailed in Sections 12.3.1 and 12.3.3 can be applied to evaluate effective properties. Gradient-based optimization requires previous knowledge of some derivatives, whose calculation is sketched below.

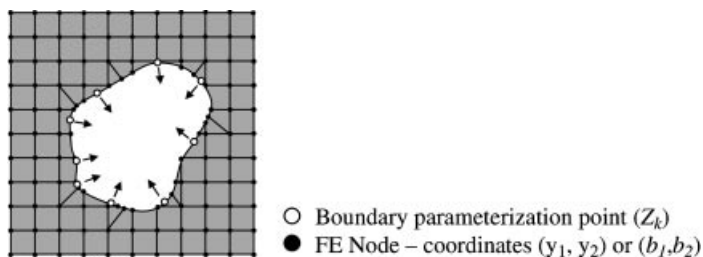


Figure 12.5 Shape optimization of a periodic cell.

Shape Sensitivity Analysis To solve the shape optimization problem it is necessary to calculate the sensitivity of homogenized properties with respect to the shape design variables Z_k . The most usual approach in the literature obtains derivatives adopting a material derivative strategy on the continuum equations, and the sensitivity expressions are subsequently discretized [42,57–60]. However, in this work, the sensitivity formulation is described considering differentiation of the discretized equations. The procedure presented is restricted to linear analyses. Nonlinear extensions can be found in Ref. [60].

We first develop the derivatives of $\mathbf{C}$, $\hat{\mathbf{R}}^{(p)}$ and $\mathbf{Q}^{(p)}$. Differentiating Eq. (12.25) with respect to an arbitrary nodal coordinate b_j ,

$$\mathbf{C} \frac{d\hat{\mathbf{R}}^{(p)}}{db_j} = \frac{d\mathbf{Q}^{(p)}}{db_j} - \frac{d\mathbf{C}}{db_j} \hat{\mathbf{R}}^{(p)} \quad (12.28)$$

From Eq. (12.27), by defining $\mathbf{B} = \nabla_y \mathbf{N}$, and considering a mapping to a master finite element with local coordinates $\xi_1 \times \xi_2$, we get

$$\mathbf{C}^e = \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \mathbf{k}^e \mathbf{B} |J| d\xi_1 d\xi_2; \quad \mathbf{Q}^{e(p)} = \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \mathbf{k}^{e(p)} |J| d\xi_1 d\xi_2 \quad (12.29)$$

so that

$$\begin{aligned} \frac{d\mathbf{C}^e}{db_j} &= \int_{-1}^1 \int_{-1}^1 \frac{d\mathbf{B}^T}{db_j} \mathbf{k}^e \mathbf{B} |J| d\xi_1 d\xi_2 + \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \mathbf{k}^e \frac{d\mathbf{B}}{db_j} |J| d\xi_1 d\xi_2 \\ &\quad + \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \mathbf{k}^e \mathbf{B} \frac{d|J|}{db_j} d\xi_1 d\xi_2 \end{aligned} \quad (12.30)$$

and

$$\frac{d\mathbf{Q}^{e(p)}}{db_j} = \int_{-1}^1 \int_{-1}^1 \frac{d\mathbf{B}^T}{db_j} \mathbf{k}^{e(p)} |J| d\xi_1 d\xi_2 + \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \mathbf{k}^{e(p)} \frac{d|J|}{db_j} d\xi_1 d\xi_2 \quad (12.31)$$

The evaluation of $d\mathbf{B}/db_j$ and $d|J|/db_j$ can be done following the *exact semi-analytical approach*, suggested by Olhoff *et al.* [61].

Now, concerning $\mathbf{k}^H$ sensitivity, from Eqs. (12.19) and (12.24) we have

$$\mathbf{k}^H = \mathbf{A}_{c=1}^N \mathbf{k}_H^e \quad (12.32)$$

$$\mathbf{k}_H^e = \frac{1}{|Y|} \int_{-1}^1 \int_{-1}^1 \mathbf{k}^e [\mathbf{I} + \mathbf{B} \hat{\mathbf{R}}] |J| d\xi_1 d\xi_2 \quad (12.33)$$

where, in the case of 2D problems

$$\hat{\mathbf{R}} = \begin{bmatrix} \hat{\mathbf{R}}^{(1)} & \hat{\mathbf{R}}^{(2)} \end{bmatrix} \quad (12.34)$$

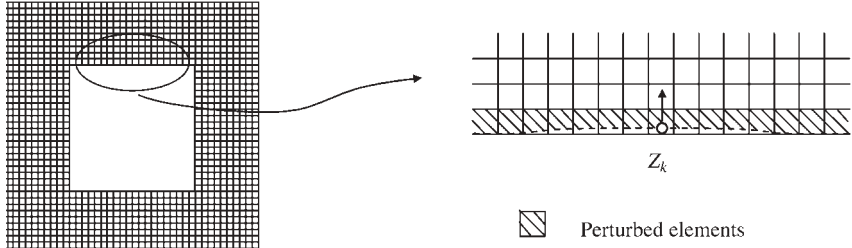


Figure 12.6 Boundary layer domain parameterization.

Using the chain rule to differentiate $\mathbf{k}^H$ with respect to the design variable Z_k , we get

$$\frac{\partial \mathbf{k}_H^e}{\partial Z_k} = \frac{\partial \mathbf{k}_H^e}{\partial b_j} \frac{db_j}{dZ_k} \quad (12.35)$$

$$\frac{\partial \mathbf{k}^H}{\partial Z_k} = A_{e=1}^N \frac{\partial \mathbf{k}_H^e}{\partial Z_k} \quad (12.36)$$

where db_j/dZ_k is the velocity field, which depends on the domain parameterization with respect to the boundary [62,63]. Notice that the first term on the right-hand side of Eq. (12.35) needs only to be calculated for nodes affected by a perturbation on Z_k . Hence, a convenient velocity field (with local effect) can be adopted in order to provide an efficient computation. One such velocity fields is given by the boundary layer approach, which considers that only the elements attached to the boundary are affected by a perturbation on the geometry (see Figure 12.6).

Differentiating Eq. (12.33) with respect to b_j provides

$$\begin{aligned} \frac{\partial \mathbf{k}_H^e}{\partial b_j} = & \frac{1}{|Y|} \int_{-1}^1 \int_{-1}^1 \mathbf{k}^e \frac{\partial \mathbf{B}}{\partial b_j} |\mathbf{J}| d\xi_1 d\xi_2 \hat{\mathbf{R}} + \frac{1}{|Y|} \int_{-1}^1 \int_{-1}^1 \mathbf{k}^e \mathbf{B} |\mathbf{J}| d\xi_1 d\xi_2 \frac{\partial \hat{\mathbf{R}}}{\partial b_j} \\ & + \frac{1}{|Y|} \int_{-1}^1 \int_{-1}^1 \mathbf{k}^e [\mathbf{I} + \mathbf{B} \hat{\mathbf{R}}] \frac{\partial |\mathbf{J}|}{\partial b_j} d\xi_1 d\xi_2 \end{aligned} \quad (12.37)$$

An alternative approach to compute directly $\partial \mathbf{k}_H^e / \partial Z_k$ uses finite differences, so that

$$\frac{\partial \mathbf{k}_H^e}{\partial Z_k} \simeq \frac{\mathbf{k}_H^e(Z + \Delta Z_k) - \mathbf{k}_H^e(Z)}{\Delta Z_k} \quad (12.38)$$

In this case, a perturbation is applied to the boundary parameterization variable, and a new perturbed mesh with the same topology is generated. $\mathbf{k}_H^e(Z + \Delta Z_k)$ is,

therefore, evaluated by

$$\mathbf{k}_H^e(\mathbf{Z} + \Delta\mathbf{Z}_k) = \frac{1}{|\mathbf{Y}|} \int_{-1}^1 \int_{-1}^1 \mathbf{k}^e[\mathbf{I} + \mathbf{B}(\mathbf{Z} + \Delta\mathbf{Z}_k)\hat{\mathbf{R}}(\mathbf{Z} + \Delta\mathbf{Z}_k)] \\ |\mathbf{J}(\mathbf{Z} + \Delta\mathbf{Z}_k)| d\xi_1 d\xi_2 \quad (12.39)$$

In practice, the presence of $\hat{\mathbf{R}}(\mathbf{Z} + \Delta\mathbf{Z}_k)$ in the expression renders this approach impractical due to the cost of recalculating Eq. (12.25).

12.3.4.2 Topology Optimization

A major concept in topology optimization is the extended design domain, which is a large fixed domain that must contain the whole structure to be determined by the optimization procedure. The objective is to determine the holes and connectivities of the structure by adding and removing material in this domain. Because the extended domain is fixed, the finite element model is not changed during the optimization process, which simplifies the calculation of derivatives of functions defined over the extended domain. In the case of the material design, the extended design domain is the unit cell domain.

However, the discrete problem, where the amount of material in each element can assume only values equal to either one or zero (that is, void or solid material, respectively), is ill-posed. A typical way to seek a solution for topology optimization problems is to relax the problem by allowing the material to assume intermediate property values during the optimization procedure, which can be achieved by defining a special material model [64]. Essentially, the material model approximates the material distribution by defining a function of a continuous parameter (design variable) that determines the mixture of basic materials throughout the domain. In this sense, the relaxation yields a continuous material design problem that no longer involves a discernible connectivity. A topology solution can be obtained by applying penalization coefficients to the material model to recover the 0–1 design (and thus, a discernible connectivity), and some gradient control on material distribution, such as a filter [65].

It turns out that this relaxed problem is strongly related to the FGM design problem, which essentially seeks a continuous transition of material properties [66]. Thus, while the 0–1 design problem needs complexity control and does not admit intermediate values of design variables, the FGM design problem does not need complexity control and does admit solutions with intermediate values of the material field.

Early work on material design followed a traditional topology optimization formulation, where the design variables are defined in a piecewise fashion in the discretized domain, which means that continuity of the material distribution is not realized between finite elements. However, considering that the topology optimization results in a smoothly graded material, a more natural way of representing the material distribution emerges by considering a continuous representation of material properties [29,67], which is achieved by interpolating the properties inside the finite element using shape functions [29,68]. The concept of employing continuum interpolation of material distribution inside the finite element is not new among the

topology optimization community; actually this concept has been implemented to model FGMs originating the so-called graded finite element [30]. Thus, nodal design variables are defined rather than the usual element-based design variables.

In the concept of the continuum distribution of design variable based on the CAMD method [29,67] the material properties are considered for each node, and the pseudo-density inside each finite element is given by

$$\rho(x) = \sum_{I=1}^{n_d} \rho_I N_I \quad (12.40)$$

where ρ_I is the nodal design variable, N_I is the finite element shape function that must be selected to provide non-negative values of the design variables and n_d is the number of nodes in each element (for example, four in the 2D case). This formulation allows a continuous distribution of material along the design domain instead of the traditional piecewise material distribution applied by previous formulations of topology optimization, and thus it is closely related to the FGM concept.

Material Model FGMs represent the transition between two basic materials, and the objective is to find the optimal volume fraction of this mixture at each point of the domain, so the FGM property gradation inside the unit cell can also be found. To achieve this, we will allow for intermediate materials (no penalization), and to guarantee that the final composite can be achieved by a mixture of chosen basic materials, a material model based on the Hashin and Shtrikman bounds is employed [51,65]. These bounds provide the range of effective properties achievable for a certain volume fraction of the mixture of two isotropic materials.

Thus, considering the upper and lower limits of thermal conductivity property (k), the material model is defined as [65]

$$k^m(\rho) = \kappa k_{\max}(\rho) + (1 - \kappa)k_{\min}(\rho) \quad (12.41)$$

where ρ is the pseudo-density describing the amount of material at each point of the domain and can assume values between 0 and 1. The parameter κ is an interpolation factor which defines a curve interpolating the upper and lower limits of the thermal conductivity property. In this work κ is assumed 0.5. The parameter k^m is the thermal conductivity modulus of the mixture. The basic materials of the mixture are designated by the symbols (+) and (-). They have thermal conductivity moduli equal to k^+ and k^- , in a way that $k^+ > k^-$. For ρ equal to 0 the material is equal to material (-) and for ρ equal to 1 the material is equal to material (+). The parameters $k_{\max}$ and $k_{\min}$ are the upper and lower limits of these moduli, and are given by [48]

$$\begin{aligned} k_{\max} &= \rho k^+ + (1 - \rho)k^- - \frac{(1 - \rho)\rho(k^+ - k^-)^2}{(1 - \rho)k^+ + \rho k^- + k^+} \\ k_{\min} &= \rho k^+ + (1 - \rho)k^- - \frac{(1 - \rho)\rho(k^+ - k^-)^2}{(1 - \rho)k^+ + \rho k^- + k^-} \end{aligned} \quad (12.42)$$

Topology Sensitivity Analysis To solve the topology optimization problem it is necessary to calculate the sensitivity of homogenized properties with respect to the design variables ρ_I . This sensitivity is well known in the literature [34–36]; however, in this section the formulation is described considering the concept of the CAMD [29].

By differentiating Eq. (12.21) with respect to the design variable ρ_I and considering Eq. (12.17), after some algebraic manipulation, one gets [34,35]

$$\frac{\partial \mathbf{k}^H}{\partial \rho_I} = \frac{1}{|Y|} \int_Y [I + \nabla_Y \mathbf{R}(\mathbf{x}, \mathbf{y})]^T \frac{\partial \mathbf{k}^m(\mathbf{x}, \mathbf{y})}{\partial \rho_I} [I + \nabla_Y \mathbf{R}(\mathbf{x}, \mathbf{y})] dY \quad (12.43)$$

However, considering the material model given by Eq. (12.41),

$$\frac{\partial \mathbf{k}^m}{\partial \rho_I} = \frac{\partial \mathbf{k}^m}{\partial \rho} \frac{\partial \rho}{\partial \rho_I} \quad (12.44)$$

and the continuous distribution of the design variable ρ_I given by Eq. (12.40), inside each finite element the pseudo-density is

$$\rho(\mathbf{x}) = \sum_{I=1}^{n_d} \rho_I N_I \Rightarrow \frac{\partial \rho}{\partial \rho_I} = N_I(\mathbf{x}) \quad (12.45)$$

By discretizing the domain into finite elements, the above integral will include all m_I elements associated with the I th node, thus:

$$\frac{\partial \mathbf{k}^H}{\partial \rho_I} = \frac{1}{|Y|} \sum_{e=1}^{m_I} \left\{ \int_{\Omega_e} [I + \nabla_Y \mathbf{R}(\mathbf{x}, \mathbf{y})]^T N_I(\mathbf{x}) \frac{\partial \mathbf{k}^m(\mathbf{x}, \mathbf{y})}{\partial \rho} [I + \nabla_Y \mathbf{R}(\mathbf{x}, \mathbf{y})] d\Omega_e \right\} \quad (12.46)$$

Thus, the calculation of gradients is straightforward and fast (low computational cost) which contributes to the efficiency of the optimization. The calculation of sensitivity $\partial \mathbf{k}^m / \partial \rho$ is obtained by differentiating Eq. (12.41).

12.4

General Applications Review

The literature shows a wide variety of modeling approaches to numerical simulation of heat transfer in cellular structures. In the context of heat transfer and fluid flow analysis, cellular materials can be regarded as porous media (metal foams), multi-finned channels (metal honeycombs), lattice structures, louvered fins and packed beds [68]. Many authors address heat transfer and pressure drop aspects in this class of problems without, however, using any optimization procedure. Detailed

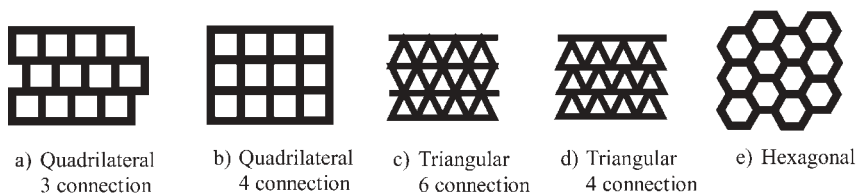


Figure 12.7 Cell morphology [15,16].

description of such models is beyond the scope of this chapter and the reader is referred to the recent publications [1,4,5,69–76], and references therein, for a better physical and numerical/analytical insight of the problem. This section highlights some relevant work on the application of optimization techniques to finding the optimum thermal design of cellular structures. Some aspects of heat transfer in multi-finned channels (primarily used as heat sinks in electronic applications) are also discussed within the cellular structure framework.

A design procedure for 2D cellular materials for combined heat dissipation and structural load capacity was presented by Gu *et al.* [15]. The authors' target is to determine the cell shape, size and arrangement that simultaneously optimize the structural and heat transfer performance at minimum weight. The cell arrangements analyzed by the authors are depicted in Figure 12.7. Two analytical models were proposed to approach heat conduction and convection in the honeycomb: the so-called corrugated wall model and the effective medium model. The former is based on analytical solutions for fin-like surfaces, whereas the latter uses a homogenization strategy to account for the combined effect of heat conduction and convection. The heat convection coefficient was obtained from Nusselt numbers available in the literature for the selected channel shape. The expression for the pressure drop was derived from the standard Hagen–Poiseuille equation for laminar flow in closed channels. The maximum thermal efficiency for both cases was defined by analytical nondimensional scaling indices which co-relate the total dissipation rate and pressure drop, with a general form given by

$$I_1 = \left(\frac{\nu_f \Omega_f u_0}{k_s} \right) \frac{\bar{h}}{\Delta p} \quad (12.47)$$

where ν_f and Ω_f are the kinematic viscosity and specific mass of the fluid, u_0 is the inlet velocity, k_s is the thermal conductivity of the walls, $\bar{h}$ is the overall heat transfer coefficient and Δp is the pressure drop. The optimization procedure consists of finding the *relative density* (array density divided by solid cell wall density), which maximizes the efficiency index for each type of cell morphology. The relative density was assumed to have a uniform distribution at the channel cross-section. The authors concluded that the regular hexagonal system produces the best heat transfer efficiency, at specified relative density, cell size and heat sink dimensions.

The structural analysis uses a stiffness index, G/E_s , based on the ratio of the in-plane shear modulus, G , and Young's modulus of the solid material, E_s . The authors emphasized that triangular cells present the greatest stiffness at a specified relative density. The thermomechanical optimization combines both heat dissipation and stiffness indices,

$$I_2 \equiv \left(\frac{G}{E_s}\right) I_1 = \left(\frac{G}{E_s}\right) \left(\frac{\nu_f \Omega_f u_0}{k_s}\right) \frac{\bar{h}}{\Delta p} \quad (12.48)$$

which presents an implicit dependence on the relative density through both G/E_s and I_1 . Gu *et al.* [15] concluded that triangular and hexagonal cells present better thermomechanical combined characteristics for small and large cell size/channel height relations, respectively.

A three-dimensional (3D) formulation aiming at designing optimum efficiency of heat dissipation in cellular structures was presented by Wang and Cheng [16]. The authors focused on the analysis of metal honeycombs with the same cell morphologies addressed by Gu *et al.* [15] (see Figure 12.7). Wang and Cheng [16] used topology optimization techniques to find the optimum design of material distribution within the cross-section of a heat exchanger for maximization of the heat dissipation efficiency. Under the total material volume constraint, both *relative density* and *local cell size distribution* were optimized. This approach allows graded honeycombs with cells of different sizes. The heat transfer equation was derived based on the concept of a mesostructural model and homogenization, so that

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) - h \alpha_A [T - T_f(z)] = 0 \quad \text{and} \quad \frac{\partial T_f}{\partial z} = \frac{Q}{c_p \rho_f v_0 S} \quad (12.49)$$

where ρ_f denotes the specific mass, h is the convection coefficient, T_f is the average fluid temperature at a given cross section, Q is the heat dissipation rate of the fluid, S is the area of the structural cross section, c_p is the specific heat, α_A is the surface area density, v_0 is the nominal velocity of the fluid flow and k_x and k_y are the homogenized thermal conductivity in x and y directions:

$$k_x = \zeta_x \rho_i k_s + (1 - \rho_i) k_f \quad \text{and} \quad k_y = \zeta_y \rho_i k_s + (1 - \rho_i) k_f \quad (12.50)$$

in which ζ_x and ζ_y are proportionality coefficients accounting for the tortuous shape of the cell walls, k_f and k_s are the thermal conductivity of the cell wall and fluid respectively and ρ_i is the local relative density. In addition, the pressure drop, Δp , was computed using the global formulas for laminar fluid flow in cylinders. Equation (12.49) was solved using finite elements with the design domain discretized with quadrilateral elements. The formulation of optimum topology design accounted for the dissipation performance of the structure, which was gauged by the ratio of total dissipation rate from the structure to the pressure drop. The target was to design the topology of cellular materials that produce high dissipation rates associated with low pressure

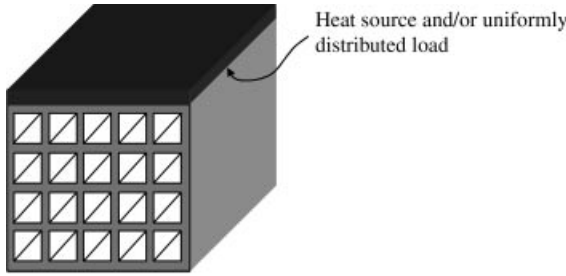


Figure 12.8 Compact heat exchanger with rectangular cellular material [3].

drops. The authors concluded that, by grading cell sizes, efficiency can increase by as much as 80% when compared to cellular materials with uniform cell sizes and shapes.

Seepersad *et al.* [3] presented a comprehensive design procedure of prismatic cellular materials combining *heat transfer* (rate of steady-state heat transfer) and *structural* (overall buckling load and structural elastic stiffness) requirements. The prismatic cells were optimized with respect to the cell aspect ratio and sizes and the authors envisaged application to compact electronic cooling devices and ultralow-weight, actively cooled and aerospace structures, which also serve structural function, as illustrated in Figure 12.8. Both finite volumes and finite elements were employed to solve the heat transfer problem. The former used a finite difference approximation for a 3D approach, whereas the latter was based on a 2D finite element discretization. The authors used homogenization considerations to account for the fluid flow and solid walls. Homogenization was performed for each single cell and not a group of cells and the heat removed by the fluid flow was included in the model as a heat sink. The structural problem is modeled using two separate approaches: structural elastic stiffness and overall buckling load. The structural elastic stiffness analysis maximizes the approximate stiffness in x and y directions, $\tilde{E}_x$ and $\tilde{E}_y$,

$$\frac{\tilde{E}_x}{E_s} \cong \frac{t_H(N_V + 1)}{H} \text{ and } \frac{\tilde{E}_y}{E_s} \cong \frac{t_V(N_H + 1)}{W} \quad (12.51)$$

where E_s is the elastic modulus of the solid cell wall material, W and H are the total width and height of the structure, t_H and t_V the horizontal and vertical wall thickness and N_H and N_V are the number of horizontal and vertical channels. The structural optimization based on the overall buckling load maximizes the critical load which was determined using the commercial finite element code ABAQUS associated with an eigenvalue buckling analysis with the cell walls modeled using Euler–Bernoulli beam elements. The *size optimization* problem is solved using a *sequential quadratic programming* algorithm in which the design variables are: number and thickness of horizontal and vertical cells, internal height of each row of cells and total mass flow rate. The authors emphasized that the multifunctional design approach is able to design families or Pareto sets of nonuniform, graded prismatic cellular materials that embody a range of tradeoffs between conflicting thermal and structural

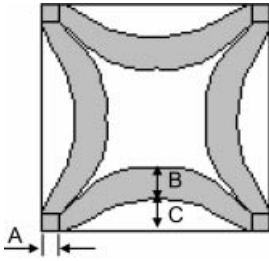


Figure 12.9 Unit cell and design variables adopted by Takano and Zako [10].

performance objectives. For instance, by defining greater weight to structural features, multifunctional designs have thicker walls and correspondingly improved structural properties (elastic stiffness and critical buckling loads), but thermal performance is sacrificed in terms of lower heat transfer rates. However, by adjusting weights and performance targets in the multiobjective decision model, the heat transfer characteristics can be improved in detriment of some structural properties.

Takano and Zako [10] proposed a genetic algorithm approach to optimize the FGM microstructure of a plate which should not warp due to prescribed different temperatures on its upper and lower surfaces. In order to show the idea, they simplified the problem, considering it one-dimensional, but the method can be extended to 2D or 3D. In their procedure, firstly they defined a microstructure pattern made of two materials and chose three geometrical design variables A , B and C (see Figure 12.9). These parameters were given 40 different values and the associated homogenized coefficients of the thermal expansion and conductivity tensors were calculated and stored in a database. Next, 10 of out of these 40 values were attributed to an integer chromosome yielding the possibility of 40^{10} combinations. The chromosome represents the graded microstructure through the thickness (see Figure 12.10).

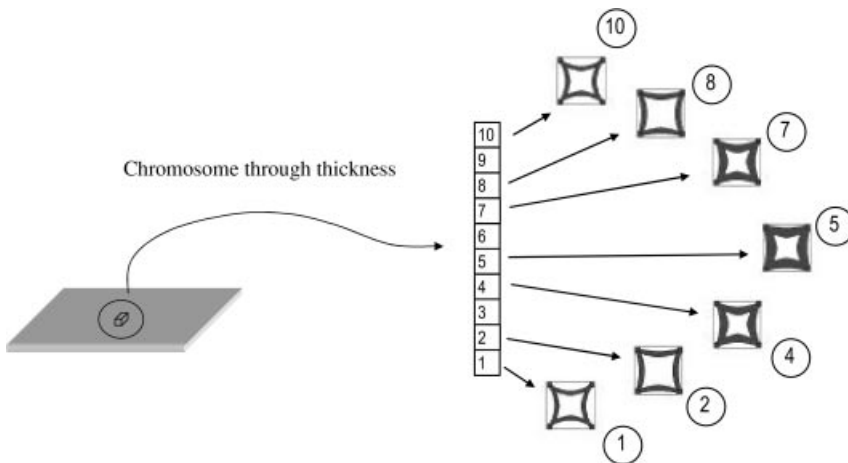


Figure 12.10 Chromosome defining the graded properties through the thickness [10].

The genetic algorithm implemented used reproduction, crossover and mutation with a population size of 100 individuals, 0.05 of mutation rate and a crossover rate between 0.6 and 0.8 [77,78]. The optimization problem was aimed to select the chromosome which best minimized the variance of the macroscopic thermal strain distribution in the thickness direction. The variance was given by

$$V_{\text{strain}} = \frac{1}{10} \sum_1^{10} (\varepsilon_n - \bar{\varepsilon}_n)^2 \quad (12.52)$$

where $\bar{\varepsilon}_n$ is the mean value of the macroscopic thermal strain distribution. The inverse of V_{strain} was used as fitness function for the GA search. An interpolation of the discrete values obtained through the thickness allowed the continuous FGM distribution.

An optimization strategy for stacked microchannel heat sinks was presented by Wei and Joshi [8] aiming at cooling electronic components. Figure 12.11 illustrates the basic design. The microchannel heat sink is attached to the electronic component and a coolant, such as water, flows in a closed-loop arrangement. The heat transfer problem was solved based on a thermal resistance network model using the heat transfer coefficient for developing laminar flow in rectangular ducts. The optimization problem consisted of minimizing the overall thermal resistance (objective function) for a maximum pressure drop and pumping power density and a given flow rate. The design variables were the fin thickness, the ratio of channel width to the fin thickness and the channel aspect ratio. The procedure used a *genetic algorithm* based on the *COMPLEX* optimization method. This method is a sequential technique that, according to the authors, has proven effective in solving problems with nonlinear objective functions. The initial sets of points are randomly scattered throughout the feasible region with the subsequent sets selected according to the *COMPLEX* method. The authors concluded that the shorter the channel, the smaller the thermal resistance for the optimized microchannel. Furthermore, the parametric study indicated that the optimal number of layers for a microchannel under constant pumping power of 0.01 W is 3.

It is relevant to mention that many solutions for heat sinks using optimization procedures can be found in the literature. However, most works adopted basic

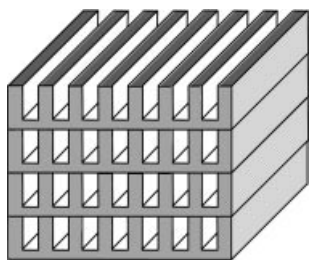


Figure 12.11 Stacked microchannel heat sink [8].

designs with a single set of finned surfaces or microchannels, which may not be strictly regarded as cellular materials. Therefore, this work will not address this class of problems and further reading may be found in [79–84].

In the design and optimization of micro heat exchangers (μ HEXs), Foli *et al.* [85], based on a genetic algorithm, studied the optimal design parameters of the μ HEX that maximizes the heat transfer rate subject to specific design constraints. The goal was to find the optimal shape of separators that simultaneously maximize the heat transfer and minimize the pressure drop in the μ HEX. The design variables were the control points of two NURBS representing part of the shape of the μ HEX. The formulations can be considered as a multiobjective optimization problem [7], since there are two conflicting objectives with opposite trends: maximize the heat transfer and minimize pressure drop in the hot gas channel and in the cold gas channel.

Jeevan *et al.* [9] studied the optimal dimensions for a stacked microchannel using genetic algorithms under different flow conditions. The physical parameters such as fin thickness, channel width, channel length, number of layers and aspect ratio of the microchannel heat sink affect the thermal resistance. These parameters were used as design variables in a genetic algorithm with pumping power density, pressure drop, flow rate, length of heat sink, width of heat sink and height of a single layer of a heat sink as constraints. The results suggested that, with a fixed pumping power and a fixed number of layers, short channels instead of long channels should be used to get lower thermal resistance. That is, if the surface to be cooled is large, several microchannel heat sinks with short channels should be used instead of a single one with long channels.

In a different approach, Haslinger and Dvorak [12] implemented a method combining shape optimization and homogenization for the identification of periodic microstructures with prescribed effective conductivities. Their procedure considered mixing two heat conducting, isotropic materials in a periodic cell made up of a matrix containing a single star-shaped inclusion, whose boundary contour is to be found. The shape sensitivities were calculated using the material derivative approach and the optimization problem was solved employing an SQP algorithm. Additional results on this work are given in [42]. Figure 12.12 illustrates the pattern of the results obtained. Dvorak further developed an *a posteriori* error estimate for the

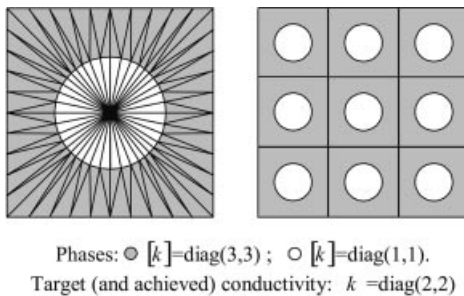


Figure 12.12 Pattern of periodic cell similar to the one used by Haslinger and Dvorak [12].

numerical homogenized coefficients and proposed to apply a p-adaptive refinement in the finite element mesh of the microstructure cell in order to achieve reliable results [45].

Barbarosie [43,44] performed shape optimization for both heat conduction and linear elasticity properties, considering a periodic cell with either inclusions or voids. He developed a special finite element mesh in order to deal with periodicity and allow more generality in the final inclusion/void shape. Although he recommended use of Bézier curves to define the boundary with few parameters, for simplicity nodal coordinates were adopted as design variables. The sensitivity was obtained via the material derivative approach [57] and the optimization problem was solved using a steepest descent implementation.

A computational approach to optimization of *functionally graded* metallic foams aiming at insulation purposes was presented by Zhu *et al.* [28]. The objective of the optimization was to ensure that the maximum temperature in the structural mass is below a specified limit. A constrained nonlinear optimization procedure was used to solve the optimization problem based on the SQP method. The authors presented one-dimensional solutions for both steady-state and transient heat transfer cases. The optimization problem for the steady-state model consisted of finding the solidity profile (or volume fraction of the foam) which maximizes the hot-side temperature of insulation (which is equivalent to minimizing the heat flux into the insulation) subjected to a constant heat flux. Simulations pointed to smaller volume fractions near the cooler side and larger volume fractions near hotter side of the metal foam for the steady-state case. However, the authors emphasized that such design does not yield good insulation performance for a transient analysis. In this case, a two-layer insulation model with constant solidity was proposed, so that each layer is optimized by varying individual solidity and thickness for a known total thickness and mass. The basic one-dimensional heat transfer equation is

$$\frac{\partial}{\partial x} \left(k_d \frac{\partial T}{\partial x} \right) = \rho_d c_p \frac{\partial T}{\partial t} \quad (12.53)$$

in which T is temperature, t is time, k_d is the thermal conductivity of the insulation layer and ρ_d and c_p are the corresponding specific mass and specific heat. Solution of Eq. (12.53) is obtained by an explicit finite difference scheme. It was found that the cooler inner layer of the optimal design has high solidity, while the hotter outer layer has low solidity. Figures 12.13a and b illustrate the optimum design for steady-state and transient analyses respectively.

12.5

Results Obtained with the FGM Approach in this Work

The objective of the present example is to design an FGM thermal conduction composite to achieve high thermal conductivity property for a certain volume fraction and to analyze the influence of gradation in the design of FGM materials using the concept

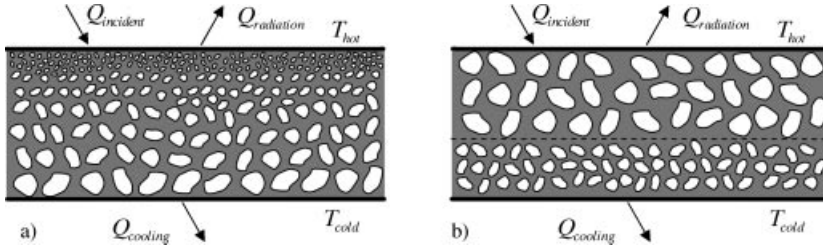


Figure 12.13 Functionally graded metal foams [28].
(a) Continuous gradation (steady state); (b) two-layer with constant solidity (transient).

of the relaxed problem in continuum topology optimization. A related analysis was performed by Hyun and Torquato [13] but restricted to non-FGMs. Their results, aiming to design multifunctional materials with high shear resistance and heat conductivity properties, led to Kagomé-like lattice structures. By introducing FGMs, the present approach can potentially design materials that achieve better performance, thus being better suited for multifunctional applications including heat-dissipation characteristics. The problem is posed as maximizing the homogenized thermal conductivity properties. A continuum distribution of the design variable inside the finite element domain is considered allowing representation of a continuous material during the design process. Since we are interested in solutions with a continuous distribution of material, we allow for intermediate materials (no penalization). The material model described in Section 12.3.4.2 is employed. A gradient control constraint in the unit cell domain is implemented based on the projection by Guest *et al.* [86]. This gradient control capability permits one to address the influence of FGM gradation in the design of extreme materials. It also avoids the problem of mesh dependency in the topology optimization implementation [65]. The actual optimization problem is solved by the *sequential linear programming* algorithm.

The optimization problem consists of maximizing a cost function related to the density distribution inside the unit cell subjected to a constraint on the material volume of phase (+). Thus, the optimization problem can be stated in continuous form as follows [31]:

$$\begin{aligned}
 &\text{Maximize} && w_1 \alpha_{11}^H + w_2 \alpha_{22}^H \\
 &\quad \rho(\mathbf{x}) \\
 &\text{Such that} && \text{Homogenization equations} \\
 &&& \int_Y \rho \, dY \leq V_0 \\
 &&& 0 \leq \rho(\mathbf{x}) \leq 1 \\
 &&& \text{Gradation control}
 \end{aligned}$$

where $\rho(\mathbf{x})$ is the pseudo-density distribution function along the unit cell domain, $\mathbf{x}$ is a position vector, α_{11}^H and α_{22}^H are the homogenized thermal conductivity properties to be maximized, and w_1 and w_2 are weight coefficients to

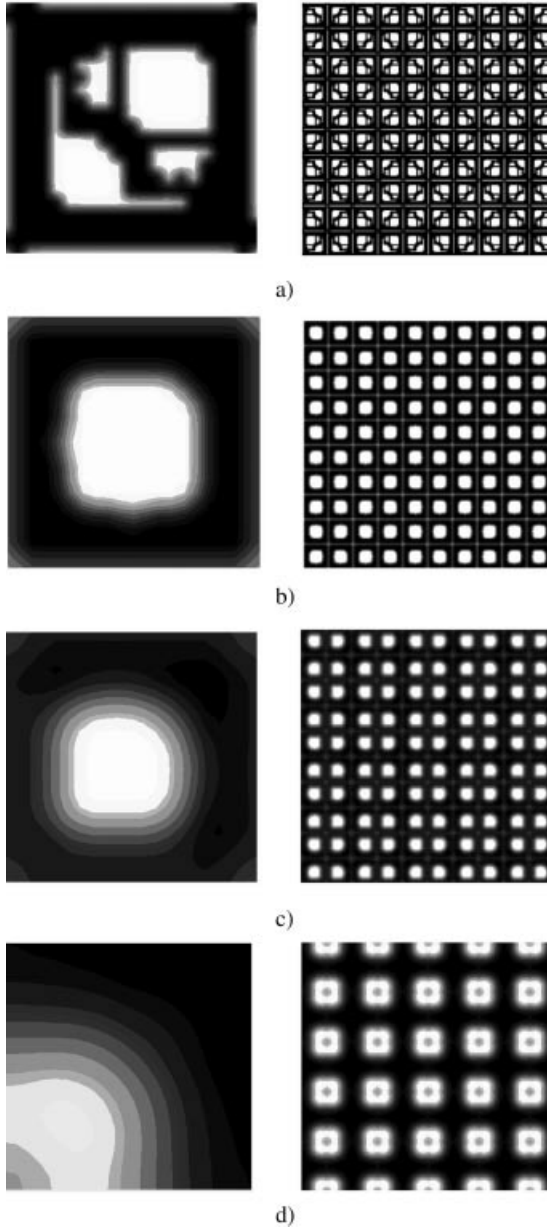


Figure 12.14 One-fourth of a unit cell pseudo-density distribution and corresponding composite material matrix:
(a) $r_{\min} = 1.1$ (almost no material gradation), $\alpha_{11}^H = \alpha_{22}^H = 0.4841$;
(b) $r_{\min} = 2$, $\alpha_{11}^H = \alpha_{22}^H = 0.4429$ (c) $r_{\min} = 4$, $\alpha_{11}^H = \alpha_{22}^H = 0.3979$;
(d) $r_{\min} = 10$, $\alpha_{11}^H = \alpha_{22}^H = 0.4032$.

control the maximization of these properties. Here emphasis is placed in 2D problems, and thus the indices i and j range from 1 to 2. The gradation control constraint is used to adjust the material gradation, and also improves aspects associated to dependency and numerical instabilities of CAMD such as *islands* phenomenon [29].

A square design domain with four symmetry axes (horizontal, vertical and both diagonals) is adopted. The symmetry conditions are implicitly expressed in the boundary conditions during the homogenization [18,19]. The symmetry ensures that the obtained composite material will be orthotropic with equal values for properties α_{11}^H and α_{22}^H . Thermal conductivity properties k^+ and k^- of basic materials are equal to 1 and 0.1, respectively. The coefficients w_1 and w_2 adopted for the objective function are both equal to -1 . The unit cell design domain is discretized into 20×20 fully integrated quadrilateral linear finite elements. The volume fraction V_0 is kept constant and equal to 60% of material (+). The minimum length required for material density change to occur is defined as $r_{\min}$ [86]. The initial values for the design variables cannot be uniform, since for a homogeneous material, equal values of gradients in relation to all design variables will be generated, and thus the optimization method does not have preferential direction for starting the search. The problem is highly dependent on the initial guess, as expected [28,31]. In the present case a random initial distribution of the design variables is used. The unit cell designs for $r_{\min}$ equal to 1.1 (almost no gradation), 2, 4 and 10 are shown in Figures 12.14a, b, c and d, respectively.

The corresponding computed property values are given in the caption to Figure 12.14. The unit cell topologies tend to a design where we have square domains of material (–) surrounded by material (+). As $r_{\min}$ increases (and thus the gradation rate), the value of effective thermal conductivity property decreases up to a value of around 0.4, then stabilizes.

12.6 Conclusions

The formulation and application of shape and topology optimization techniques to achieve enhanced conductivity properties in cellular materials has been described.

Regarding shape optimization, as opposed to the usual material derivative approach, alternative discrete shape sensitivity equations have been derived for this kind of application. Regarding topology optimization, a functionally graded material approach has been proposed in order to relax the typical 0–1 material distribution, thus allowing the consideration of porous materials. Some novel results using this approach have been presented.

A general review on the use of optimization techniques for achieving enhanced thermal properties in a wide range of engineering applications has been included.

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