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Chapter 82
Mathematical Expressions for Prediction of the Effective Thermal Conductivity of Perfectly Packed Two-Phase Mixtures

Carl-Eric Hagentoft and Ali Naman Karim

Abstract This paper introduces new and handy mathematical expressions for predicting and understanding the effective thermal conductivity of two-phase homogeneous mixtures. In a two-phase mixture, particles of the dispersed phase are mixed in the matrix of the second phase. A primary purpose of the proposed model is to predict and understand the effective thermal conductivity of high porous thermal insulation materials, for which many other similar analytical models offer less accuracy. The presented expressions assume a perfectly packed mixture and consider the thermal conductivity of the two phases, the proportion and the particle size of the dispersed phase. The proposed model includes non-dimensional heat loss factors, calculated by two and three-dimensional numerical simulations. In the continuation of the work presented, an experimental study is planned to evaluate the accuracy of the model, compared to other existing analytical solutions, and the validity of the assumptions made.

Keywords Effective thermal conductivity · Two-phase mixtures · Mathematical expressions

82.1 Introduction

The effective thermal conductivity (ETC) of two-phase mixtures has been the subject of several research studies throughout the years (Pietrak and Wiśniewski 2015). Based on these studies, many calculation models have been proposed that are mainly empirical, analytical, or numerical. For calculations based on numerical analyses, the finite difference method, finite element method and boundary element method are the common numerical methods that are used for the prediction of the ETC of such mixtures (Zhu et al. 2014). Regarding mathematical models, there are some widely used analytical methods. In (Pietrak and Wiśniewski 2015), Pietrak et al.

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present a review of these models. The Maxwell model presented the first analytical expressions for two-phase mixtures, where the spherical particles of one component, fillers, were embedded in a matrix of the second component. This model assumed no thermal interaction between the spheres, and it was proven to be valid only for mixtures with low volume fraction of fillers, up to 25%. Several new methods were later developed based upon modifications on the original Maxwell model such as the Maxwell-Eucken model, Raleigh model, Percolation model, and the Cheng and Vachon model that are also further developed and modified.

Despite the large numbers of existing models for prediction of ETC of two-phase mixtures, there is today no unique model that is used for predicting the ETC of all two-phase mixtures (Li et al. 2013). Among the existing models, there are few that are validated or sufficiently accurate for mixtures with high volume fraction of the dispersed phase. Example of such mixtures are thermal insulation materials with high porosity (air content). As an attempt to contribute to this field of research, this paper proposes simple and handy mathematical expressions intended to be used for understanding and predicting the ETC of two-phase mixtures with high volume fraction of the dispersed phase. Examples of such mixtures are high porous thermal insulation materials such as aerogel-based concretes or coating mortars. The current version of the mathematical expressions presented assumes of perfectly packed particles in the mixture and includes non-dimensional heat loss factors that are dependent on the thermal conductivity of the two phases, and the size and volume fraction of the dispersed phase. In this paper, these factors are predicted using two-dimensional (2D) and three-dimensional (3D) numerical simulations.

82.2 Methods

In this section, the derivation and the procedure of developing the mathematical expressions for the prediction of the ETC of two-phase mixtures is introduced.

82.2.1 Derivation of Equations

The mathematical expressions developed are based on analyses in 2D and 3D. Here, it is assumed that the spherical particles of the dispersed phase are perfectly and symmetrically packed in the mixture of the second phase. Furthermore, the size of all particles is assumed to be the same. Figure 82.1 illustrates the geometrical details and the defined parameters in the analysis conducted in 2D.

Equations (82.1)–(82.24) present the detailed derivation steps in 2D towards the final expression shown in (82.25). An important and often used parameter in this type of analysis is the porosity, $\varphi(-)$, which becomes:

$$\varphi = \frac{d^2\pi}{4D^2} = \frac{\pi}{4}\left(\frac{d}{D}\right)^2 \tag{82.1}$$

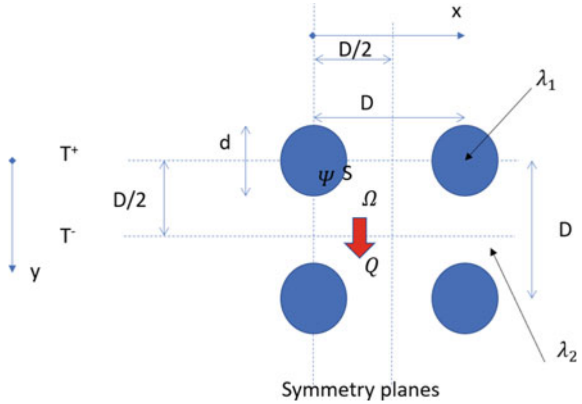

Fig. 82.1 Schematic illustration of the geometrical details and the defined parameters in the analysis

$$\frac{d}{D} = \sqrt{\frac{4\varphi}{\pi}} \tag{82.2}$$

The effective thermal conductivity (ETC), here denoted λ_{eff} (W/mK), is defined by the heat flow Q (W) over $0 < x <$ D/2 and $0 < y <$ D/2:

$$Q = \lambda_{eff} \frac{T^+ - T^-}{\frac{D}{2}} \cdot \frac{D}{2} \cdot 1 \quad = \lambda_{eff} \cdot \left(T^+ - T^-\right) \tag{82.3}$$

The effective thermal conductivity can also be obtained from the numerically calculated 2D heat flow , $q_{2D,numerical}(W/m)$, between $0 < x <$ D/2:

$$\lambda_{eff} = \frac{q_{2D,numerical}}{T^+ - T^-} \tag{82.4}$$

The steady-state heat conduction equation in the two domains, Ω and Ψ gives:

$$\frac{\partial}{\partial x}\left(\lambda_2 \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_2 \frac{\partial T}{\partial y}\right) = 0 \quad \Omega \tag{82.5}$$

$$\frac{\partial}{\partial x}\left(\lambda_1 \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_1 \frac{\partial T}{\partial y}\right) = 0 \quad \Psi \tag{82.6}$$

The continuity of heat flow at the boundary, S, between the two materials gives:

$$\lambda_2 \frac{\partial T}{\partial n} = \lambda_1 \frac{\partial T}{\partial n} \tag{82.7}$$

$$T_\Omega = T_\Psi \tag{82.8}$$

In addition, the exterior boundary conditions are:

$$T = T^+ \quad y = 0 \tag{82.9}$$

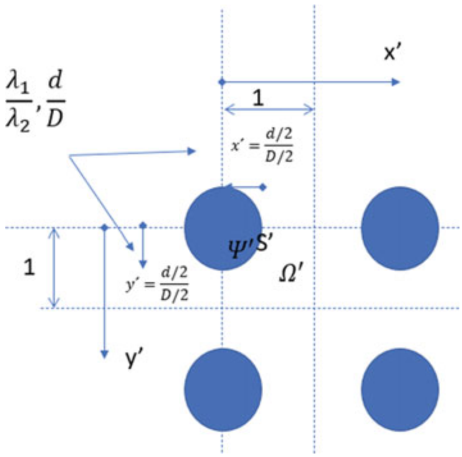

Fig. 82.2 Schematic illustration of the geometrical details and the defined parameters for the case of dimensionless formulation

$$T = T^{-} \quad y = \frac{D}{2} \tag{82.10}$$

The equations are transformed into non-dimensional form illustrated in Fig. 82.2. Scaling using the length D/2 gives:

$$x = \frac{D}{2} \cdot x' \tag{82.11}$$

$$y = \frac{D}{2} \cdot y' \tag{82.12}$$

The non-dimensional temperature u (−) is introduced:

$$T = \left(T^{+} - T^{-}\right) \cdot u\left(x', y'\right) + T^{-} \tag{82.13}$$

The heat flow over $0 < x <$ D (and the depth of 1 m in the z-direction) gives the heat flow using a two-dimensional approximation for Q:

$$Q = -1 \cdot \int_{0}^{\frac{D}{2}} \lambda_2 \left.\frac{\partial T}{\partial y}\right|_{y=\frac{D}{2}} dx \tag{82.14}$$

Using the non-dimensional formulation, the heat conduction equation reads:

$$\frac{\partial^2 u}{\partial x'^2} + \frac{\partial^2 u}{\partial y'^2} = 0 \quad \Omega \tag{82.15}$$

$$\frac{\partial^2 u}{\partial x'^2} + \frac{\partial^2 u}{\partial y'^2} = 0 \quad \Psi \tag{82.16}$$

Here u now depends on the dimensionless length coordinates x' and y'. The interior boundary condition reads:

$$\frac{\partial u}{\partial n'} = \frac{\lambda_1}{\lambda_2}\frac{\partial u}{\partial n'} \quad S' \tag{82.17}$$

$$u_\Omega = u_\Psi \quad S' \tag{82.18}$$

And the exterior boundary condition reads:

$$u = 1 \quad y' = 0 \tag{82.19}$$

$$u = 0 \quad y' = 1 \tag{82.20}$$

Using (82.14) and the non-dimensional form for the temperature solution:

$$Q = -1 \cdot \int_0^{\frac{D}{2}} \lambda_2 \left.\frac{\partial T}{\partial y}\right|_{y=\frac{D}{2}} dx = -\lambda_2\left(T^+ - T^-\right) \cdot 1 \int_0^1 \left.\frac{\partial u}{\partial y'}\right|_{y'=1} dx' = \lambda_2\left(T^+ - T^-\right) \cdot h \tag{82.21}$$

Here, h (−) is a non-dimensional heat loss factor depending on two non-dimensional parameters $\frac{\lambda_1}{\lambda_2}, \frac{d}{D}$:

$$h\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) = -\int_0^1 \left.\frac{\partial u}{\partial y'}\right|_{y'=1} dx' \quad (-) \tag{82.22}$$

Combining this with the expression for porosity (82.2) gives:

$$Q = \lambda_2\left(T^+ - T^-\right) \cdot h\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) = \lambda_2\left(T^+ - T^-\right) \cdot h\left(\frac{\lambda_1}{\lambda_2}, \sqrt{\frac{4\varphi}{\pi}}\right) \tag{82.23}$$

The limit for the geometrical dimensions gives:

$$0 \le \frac{d}{D} \le 1 \Rightarrow \frac{4\varphi}{\pi} = \left(\frac{d}{D}\right)^2 \le 1 \Rightarrow \varphi \le \frac{\pi}{4} \approx 0.7854 \tag{82.24}$$

Combined with the definition of the effective thermal conductivity (82.3) gives:

$$\lambda_{eff} = \lambda_2 \cdot h\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) \tag{82.25}$$

The analyses for the 3D case, with spheres of diameter d (m) and the closest distance to the nearest sphere D (m), can be performed in a similar fashion as for the 2D case, and is not presented in detail here. For the porosity, the relation with the dimensions becomes:

$$\varphi = \frac{\frac{4\pi d^3}{8\cdot 3}}{D^3} = \frac{\pi}{6}\left(\frac{d}{D}\right)^3 \tag{82.26}$$

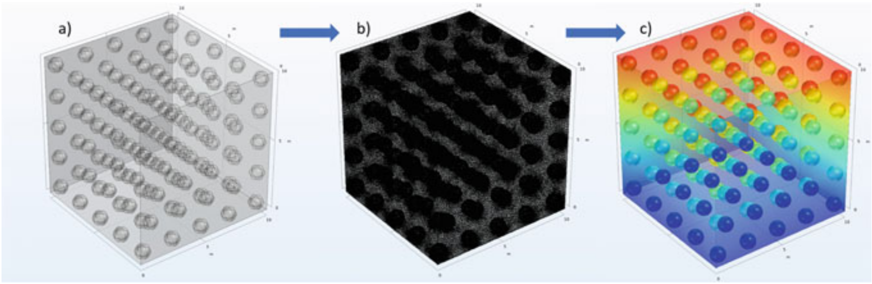

Fig. 82.3 Illustration of an example in 3D describing the calculation steps in the numerical analysis. **a** Generation of the geometry in MATLAB imported to COMSOL. **b** Meshing of the domain in COMSOL. **c** Calculation of the ETC by solving the conductive heat transfer equation

$$\frac{d}{D} = \left(\frac{6\varphi}{\pi}\right)^{\frac{1}{3}} \tag{82.27}$$

The expression for the heat loss becomes:

$$Q = \lambda_{eff} \cdot \frac{D}{2}\left(T^{+} - T^{-}\right) \tag{82.28}$$

$$\lambda_{eff} = \lambda_2 h^{*}\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) \tag{82.29}$$

Here, the non-dimensional heat loss factor from the 3D analysis is denoted by h^{*} (−). It depends on the same two non-dimensional parameters as in the 2D-case.

82.2.2 Numerical Simulation

The non-dimensional heat loss factors used in the presented mathematical expressions (h and h*) are predicted using 2D and 3D numerical finite element analyses. The full description of the conducted numerical simulations are presented in Mirzanamadi et al. Jan. (2018), Karim and Hagentoft (2022). The geometries of the samples are generated in MATLAB (R2017b) and imported to COMSOL (5.4) where the meshing and solving of the conductive heat equation is performed. Figure 82.3 shows the order of the calculation steps.

82.3 Results

Based on the analyses presented in this papers, mathematical expressions presented in (82.30) and (82.31) are proposed to predict the ETC of two-phase mixtures. The expressions include the non-dimensional heat loss factors (h and h*) based on the 2D and 3D analyses. The predicted values and the corresponding interpolation curves for a range of thermal conductivities (c: λ_1/λ_2) are presented in Fig. 82.4. As illustrated, the 2D analyses predict higher values compared to 3D. By using the Eqs. 82.30 and 82.31 and based on the fraction of the dispersed phase (d/D) and the relation between the thermal conductivity of the two phases (c: λ_1/λ_2), the ETC (λ_{eff}) of a two-phase mixture can be predicted. To illustrate an example, the ETC of an aerogel-based coating mortar with 50 vol% (d/D: 0.5) aerogel granules can be predicted. Assuming a thermal conductivity of 0.4 W/mK for the mixture and 0.022 W/mK (Karim and Hagentoft 2022) for the dispersed phase (aerogels), the heat loss factors 0.343 and 0.372 (h and h* respectively) can be read from Fig. 82.4 (c:0.055). Using (82.30) and (82.31), the ETC can be predicted to 0.137 and 0.148 W/mK respectively.

$$\frac{\lambda_{eff}}{\lambda_2} = h\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) \tag{82.30}$$

$$\frac{\lambda_{eff}}{\lambda_2} = h^*\left(\frac{\lambda_1}{\lambda_2}, \frac{d}{D}\right) \tag{82.31}$$

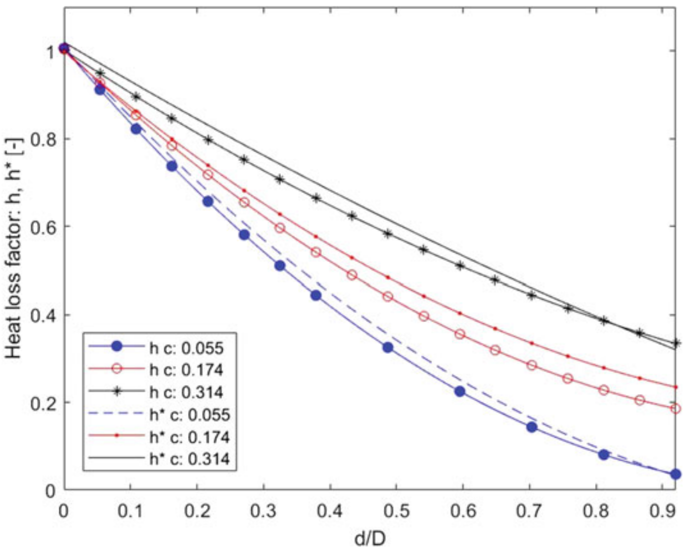

Fig. 82.4 Interpolation curves, based on numerical simulations, for the non-dimensional heat loss factors h and h*, c: λ_1/λ_2)

82.4 Discussion

The mathematical expressions presented in this paper can be used for the prediction of ETC of two-phase mixtures. The expressions include non-dimensional heat loss factors that are, in this paper, predicted based on numerical simulations in 2D and 3D. At the current stage, the accuracy of the model compared to other available analytical solutions is not examined. A comparison between the calculated and experimentally measured thermal conductivity of two-phase mixtures is required to validate the assumptions made and to state the accuracy of the model. Based on such a validation study, the model and the corresponding correlation factor can, if necessary, be further developed. Also, more numerical calculations are needed to define the non-dimensional heat loss factors for a wider range of thermal conductivities of the two phases in the mixture.

82.5 Conclusions

Handy mathematical expressions are proposed for predicting the effective thermal conductivity of two-phase mixtures based on the assumption that particles in the dispersed phase are perfectly packed in the mixture of the second phase. The proposed model incorporates the thermal conductivity of the two phases as well as the size and fraction of the particles. It also includes non-dimensional heat loss factors that are predicted based on numerical analyses. To state the accuracy of the implied model, and to validate the assumption made, an experimental study is planned to compare the calculated values with the measured thermal conductivity of two-phase mixtures.

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