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A hybrid approach on predicting the effective thermal conductivity of porous and nanoporous media

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In this paper, an analytical formula for the effective thermal conductivity of porous media saturated with two immiscible fluids is derived for a wide range of pore sizes. The method applied to derive the formulas for the effective thermal conductivity is based on the mesoscopic adaptation of the hybrid approach by taking into account the influence of different types of scattering events on the interfaces between fluids and grain phase. The influence of surface roughness on the effective thermal conductivity is explored. Analysis of the results demonstrates a very good agreement of the theoretical approach with available experimental data. It is also observed that as the surface roughness increases, the heat carrier confinement at the grain surface increases and consequently the effective thermal conductivity decreases.

1. Introduction

The effective thermal conductivity of a heterogeneous medium is an important property for various engineering applications including oil production, gas diffusion layers, polymer composites, thermoelectric materials, and soil science. In heterogeneous porous materials the effective thermal conductivity depends on the nature of their homogeneous components, morphology, porosity, degree of saturation and interface properties. However, the prediction of the thermal conductivity of these types of materials involves complicated procedures. The series model, the parallel model, the Maxwell–Eucken model and the effective medium theory (EMT) either individually or in combination are generally used to investigate the effective thermal conductivity of heterogeneous media [1].

In the series and parallel models, it is assumed that the individual components of the heterogeneous medium are in the form of layers aligned either perpendicular or parallel to the imposed temperature gradient direction. The effective thermal conductivity of a dispersion of small spherical particles in a continuous matrix can be investigated by the Maxwell model. In derivation of the Maxwell model, the spheres are considered far enough apart from each other in order not to interfere with their neighbours temperature distributions. In other words, the interaction between particles is neglected. A complete randomness of the dispersed phase is the characteristic of the effective medium theory. In addition to these models, different numerical and theoretical attempts have been made to predict the effective thermal conductivity of heterogeneous structures [2–4,1,5–9]. For instance, the fractal technique has been used to predict the permeability [10–12] and the effective thermal conductivity [7] of porous media. Ordonez-Miranda et al. have used the crowding factor model for the prediction of the thermal conductivity of a composite [13]. In another attempt to predict the effective thermal conductivity of composites, they have developed Bruggeman theory-based models [14]. Krupiczka approximated the thermal conductivity of a porous medium consisting of a bundle of long cylinders [15]. Zehner and Schlunder derived an expression to predict the effective thermal conductivity of a porous medium by assuming a unit cell of cylindrical shape with embedded spherical particles [16]. A great deal of these works have been devoted to the effective thermal conductivity of porous media saturated by only one fluid. In other words, these models are generally able to study the effective thermal conductivity of a medium consisting of two components. The hybrid approach is another method which is used to predict the effective thermal conductivity of heterogeneous media constructed by several components [2,3,8,9]. In this study, the hybrid technique is considered and extended to introduce an analytical formula for the effective thermal conductivity predictions of tight rock porous media saturated by two immiscible fluids. Results of our approach are compared against available experimental data and other theoretical models for porous media saturated with air and water. Although our model is able to predict the effective thermal conductivity in a macroscopic regime where the classical Fourier theory is valid, its applicability is limited when the size of media is in the order of nanometers [6,17–19]. If, given a porous medium, the pore size is in the order of or smaller than the mean free path of the heat

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Nomenclature

A	area
C	specific heat capacity
D_f	pore area fractal dimension
D_t	tortuosity fractal dimension
f	density function
h	thickness of the fluid layer
Kn	Knudsen number
L_t	capillary length
L_0	representative length
N	number of pores or capillaries
r_p	grain size
R	resistance
s	specularity of the surface
S_w	wetting phase saturation
t	transmission coefficient
T	temperature
v	heat carrier velocity

Subscripts

b	bulk
$cirt$	critical
$coll$	collision
eff	effective
g	grain phase
i,j	component
max	maximum
min	minimum
nw	non-wetting phase
TBR	thermal boundary resistance
w	wetting phase

Superscripts

$diff$	diffuse
$\parallel$	parallel
$\perp$	perpendicular
$spec$	specular

Greek letters

$\beta \& \beta'$	empirical parameter
Γ	gamma function
Δ'	characteristic length
Δ	volume fraction
κ	pore size
λ	thermal conductivity
Λ	mean free path
μ	$\cos\theta$
ξ	probability of the surface scattering
ρ	density
ϕ	porosity
ω	frequency

carriers then the heat conduction is studied by referring to, for instance the Boltzmann–Peierls theory (in which heat is seen as a gas of heat carriers) [20–22], hydrodynamic models [23,24] and kinetic theory. In this study the approach presented elsewhere [25,26,8,9] is extended to nanoporous media saturated by two fluids. Our aim here is to investigate the influence of the surface roughness, grain size and fluid saturation on the effective thermal conductivity of the porous media.

2. Effective thermal conductivity of porous media

2.1. Fractal technique

For many disciplines, the fractal technique is used to study the different properties such as permeability, thermal conductivity, and mass diffusivity of disordered and irregular structures. A porous medium such as a sandstone of an oil reservoir consists of a combination of numerous irregular and disordered pores of different sizes and tortuosities. For a tortuous capillary of diameter κ and tortuous length of $L_t(\kappa)$ along the transport direction, a fractal scaling relation between the diameter and length of tortuous capillaries is presented [10,27]

$$L_t(\kappa) = \kappa^{1-D_t} L_0^{D_t} \tag{1}$$

where L_0 is the representative length of the medium. Due to the tortuous nature of capillary tubes, $L_t \geqslant L_0$. By $1 < D_t < 2$ the tortuosity fractal dimension is denoted. Obviously for a straight capillary tube $D_t \to 1, L_t = L_0$. The higher is D_t, the more tortuous is the capillary tube. Size distribution of pores is another important porous medium characteristic that should be addressed. It has been shown that the cumulative size distribution of the pores can be mathematically expressed by the fractal power law [10,28],

$$N(L \geqslant \kappa) = \left(\frac{\kappa_{max}}{\kappa}\right)^{D_f} \tag{2}$$

where D_f stands for the pore area fractal dimension. κ and κ_{max} are the pore size and the maximum pore size of the porous media, respectively. The number of pores of sizes between κ to $\kappa + d\kappa$ is given by differentiating Eq. (2).

$$-dN = D_f \kappa_{max}^{D_f} \kappa^{-(D_f+1)} d\kappa \tag{3}$$

Minus in Eq. (3) represents that pore population decreases with increasing pore size. The total number of pores (from the smallest size κ_{min} to the largest size κ_{max}) can be given by Eq. (2) as

$$N_t(L \geqslant \kappa_{min}) = \left(\frac{\kappa_{max}}{\kappa_{min}}\right)^{D_f} \tag{4}$$

The probability density function $f(\kappa) = D_f \kappa_{min} \kappa^{-(D_f+1)} \geqslant 0$ is generated from dividing Eq. (3) by Eq. (3)

$$-\frac{dN}{N_t} = D_f \kappa_{min} \kappa^{-(D_f+1)} d\kappa \tag{5}$$

According to the probability theory, the probability density function should satisfy the following expression

$$\int_0^\infty f(\kappa) d\kappa = \int_{\kappa_{min}}^{\kappa_{max}} f(\kappa) d\kappa = 1 - \left(\frac{\kappa_{min}}{\kappa_{max}}\right)^{D_f} \equiv 1 \tag{6}$$

Eq. (6) is valid if and only if $\left(\frac{\kappa_{min}}{\kappa_{max}}\right)^{D_f} = 0$ [10]. This means that the fractal technique can be applied if $\kappa_{min} \ll \kappa_{max}$, otherwise the porous medium is a non-fractal medium. Although this statement is not exactly met for typical porous media $\left(\text{that is typically } \frac{\kappa_{min}}{\kappa_{max}} = 10^{-2}\right)$, it is reasonable to use the fractal theory to approximate properties of porous media [7,10]. The fractal theory is applied here to study the effective thermal conductivity of porous media saturated by two immiscible fluids. If the pore cross sections are considered as circles the total pore area is determined by the following expression