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Thermal dispersion in porous media: one-equation model

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Abstract

In this work, the methods of volume average and multiple scale expansion are employed to obtain one macroscopic equation governing thermal dispersion in a rigid homogeneous porous medium. The structure of the real porous medium is described here by a spatially periodic model. The theoretical longitudinal thermal dispersion coefficient for a stratified system is compared with numerical data obtained from a random walk method, and good agreement is achieved. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

In the macroscopic description of heat transfer in porous media, the convection-diffusion phenomena (or dispersion) in a porous medium are generally analyzed using an up-scaling method, in which the complicated local situation (the transport of energy by convection and diffusion at pore scale) is described at the macroscopic scale. At this level, the dispersion can be characterized by the *effective thermal dispersion tensor*.

There are several different ways of up-scaling for dispersion in a porous medium: among others, the method of moments [1], the volume average method [2], the homogenization method [3] and the ensemble average method [4]. In this work, we shall use the volume average and homogenization methods to obtain a one-equation model that describes the thermal dispersion in a homogeneous porous medium.

There has been some controversy in the literature [2,5] regarding the applicability of one-equation models to study the thermal dispersion in a porous medium. One-equation models often assume that the fluid and solid are both at same intrinsic average temperature $\langle T\rangle = \langle T_\beta\rangle^\beta = \langle T_\sigma\rangle^\sigma$. But as demonstrated below, this condition is impossible to achieve for this type of situation. Nevertheless, it is still possible to derive a one-equation model for the *average* temperature of the medium.

How can this *average* temperature be defined for the whole medium (that is to say, for both the β-phase and the σ-phase)? As the temperature is an intensive property from a thermodynamic point of view, it is justifiable to average an extensive property, the energy (or more precisely here the enthalpy), rather than the temperature because as we shall show further on, the mean temperature deviations are not necessarily zero. By replacing this condition with another, we can use the volume average method to get a one-equation model with a new effective thermal dispersion tensor and closure problem.

In order to demonstrate the pertinence of the physical assumptions used in deriving the one-equation model based on the volume average method, we prove

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Nomenclature

A	area
c_p	heat capacity
$\overline{\overline{D}}$	effective hydrodynamic dispersion tensor
e	thickness of solid
$\vec{f}$	vector field mapping $\nabla\langle T\rangle$ onto $\tilde{T}\beta$
$\vec{g}$	vector field mapping $\nabla\langle T\rangle$ onto $\tilde{T}\sigma$
h	thickness of fluid
H	total height of unit cell
$\mathscr{H}$	enthalpy
$\overline{\overline{I}}$	identity tensor
k	thermal conductivity
$\overline{\overline{K}}_\mathrm{eff}$	effective thermal dispersion tensor
K_{xx}	longitudinal coefficient of the effective thermal dispersion tensor
ℓ	characteristic length associated with the microscopic scale
L	characteristic length associated with local volume average quantities
$\vec{n}$	outwardly directed unit normal vector
p	probability of passage
Pe	Péclet number
Q	energy source
$\vec{r}$	vector position
t	time
t_c	characteristic time for convection
t_d	characteristic time for diffusion
T	point temperature
$\tilde{T}$	spatial deviation of the temperature
u	velocity component in the x-direction
$\vec{v}$	vector velocity
v_ref	reference velocity
V	averaging volume
x	spatial macroscopic coordinate
y	spatial microscopic coordinate

Greek symbols

α	thermal diffusivity
γ_β	ratio $\varepsilon_\beta(\rho c_\mathrm{p})_\beta/\langle\rho c_\mathrm{p}\rangle$
δ	Dirac distribution
$\vec{\delta}_\mathrm{c}$	displacement due to convection
$\vec{\delta}_\mathrm{d}$	displacement due to diffusion
δt	time step
δx	spatial displacement
δy	spatial displacement
ϵ	scale factor ($\epsilon = \ell/L$)
ε	volume fraction
ρ	density
$\overline{\overline{\tau}}$	tortuosity tensor

Subscripts, superscripts and other symbols

$\mathcal{O}()$	order of magnitude
β	fluid-phase
βe	fluid-phase entrances and exits
$\beta\sigma$	β–σ interface
$\beta\to\sigma$	from the fluid into the solid
σ	solid-phase
σe	solid-phase entrances and exits
$\sigma\to\beta$	from the solid into the fluid
$\langle\rangle$	spatial average
$\langle\rangle^\beta$	intrinsic β-phase average
$\langle\rangle^\sigma$	intrinsic σ-phase average

that the same result can be obtained using the more mathematical framework of the homogenization method.

Lastly, we compare the calculated values of the longitudinal thermal dispersion coefficient with those determined by a numerical experiment using the random walks of *thermions* for the simple case of a stratified medium for which the closure problem can be solved analytically.

2. Governing microscopic equations

The transport of energy at the pore level is described by the following equations and boundary conditions for the fluid (β-phase) and solid (σ-phase)

$$(\rho c_\mathrm{p})_\beta\frac{\partial T_\beta}{\partial t} + (\rho c_\mathrm{p})_\beta\vec{v}_\beta\cdot\nabla T_\beta = \nabla\cdot\left(k_\beta\nabla T_\beta\right) \tag{1}$$

$$(\rho c_\mathrm{p})_\sigma\frac{\partial T_\sigma}{\partial t} = \nabla\cdot(k_\sigma\nabla T_\sigma) \tag{2}$$

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \tag{3}$$

$$\vec{n}_{\beta\sigma}\cdot k_\beta\nabla T_\beta = \vec{n}_{\beta\sigma}\cdot k_\sigma\nabla T_\sigma \quad \text{at } A_{\beta\sigma} \tag{4}$$

and with appropriate initial and boundary conditions for T_β and T_α at $t = 0$ and at the area of the entrances and exits for the β-phase, $A_{\beta e}$, and for the σ-phase, $A_{\sigma e}$.

To describe the heat transfer completely, the equations of continuity and motion have to be introduced for the fluid phase. Here, we assume that the physical properties of the fluid and solid are constant. The hydrodynamic problem can then be solved independently.

3. Volume average method

To obtain the macroscopic equation, we use the average volume method [2]. In this method, the macroscopic quantities are regularized spatial fields obtained by spatial averaging of the microscopic quantities at the pore level. In the literature, we see how these macroscopic quantities, free of the fluctuations associated with the small-scale, can be obtained for ordered and disordered systems from an appropriate choice of weighting functions [5].

For practical purposes, we will use a spatially periodic porous medium as model, i.e. the whole medium can be generated by translating a unit cell of arbitrary shape in three independent directions of space. For this reason, we shall use the usual definitions of the average volume method as we consider only periodic systems here.

Two volume averages are employed in this paper: the first is the phase average, defined by

$$\langle \psi_{\beta,\sigma} \rangle = \frac{1}{V}\int_{V_{\beta,\sigma}} \psi_{\beta,\sigma}\,\mathrm{d}V. \tag{5}$$

and the second is the intrinsic phase average

$$\langle \psi_{\beta,\sigma} \rangle^{\beta,\sigma} = \frac{1}{\varepsilon_{\beta,\sigma}}\langle \psi_{\beta,\sigma} \rangle = \frac{1}{V_{\beta,\sigma}}\int_{V_{\beta,\sigma}}\int_{V_{\beta,\sigma}} \psi_{\beta,\sigma}\,\mathrm{d}V \tag{6}$$

The first average is the quantity that appears in the averaging theorem

$$\langle \nabla\psi_{\beta,\sigma} \rangle = \nabla\langle \psi_{\beta,\sigma} \rangle + \frac{1}{V}\int_{A_{\beta\sigma}} \psi_{\beta,\sigma}\vec{n}_{\beta\sigma}\,\mathrm{d}A \tag{7}$$

or in the divergence form

$$\langle \nabla\cdot\psi_{\beta,\sigma} \rangle = \nabla\cdot\langle \psi_{\beta,\sigma} \rangle + \frac{1}{V}\int_{A_{\beta\sigma}} \psi_{\beta,\sigma}\cdot\vec{n}_{\beta\sigma}\,\mathrm{d}A \tag{8}$$

for a $\psi_{\beta,\sigma}$, vector or tensor defined in the β or σ phase.

3.1. *Average temperature of the medium*

Based on the arguments described in the introduction, the average temperature of the medium is introduced by averaging the enthalpy. Using $\mathscr{H}$ to designate the enthalpy per unit mass, the definition of the average enthalpy of the medium is clearly given by:

$$\langle\rho\rangle\langle\mathscr{H}\rangle = \varepsilon_\beta\rho_\beta\langle\mathscr{H}_\beta\rangle^\beta + \varepsilon_\beta\rho_\sigma\langle\mathscr{H}_\sigma\rangle^\sigma \tag{9}$$

with $\langle\rho\rangle = \varepsilon_\beta\rho_\beta + \varepsilon_\sigma\rho_\sigma$.

Considering the calorimetric equation for each phase (for example, $\mathscr{H}_\beta = c_{\mathrm{p}\beta}T_\beta$) and postulating the same type of relation for the whole medium, the average temperature $\langle T\rangle$ is then defined by:

$$\begin{aligned}\langle\rho\rangle\langle c_\mathrm{p}\rangle\langle T\rangle &= \langle\rho c_\mathrm{p}\rangle\langle T\rangle\\ &= \varepsilon_\beta(\rho c_\mathrm{p})_\beta\langle T_\beta\rangle^\beta + \varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\langle T_\sigma\rangle^\sigma.\end{aligned} \tag{10}$$

Requiring that the average temperature $\langle T\rangle$ is equal to the temperature of both phases in the case of the thermal equilibrium ($\langle T_\beta\rangle^\beta = \langle T_\sigma\rangle^\sigma$), we get the definition of the heat capacity per unit volume:

$$\langle\rho c_\mathrm{p}\rangle = \varepsilon_\beta(\rho c_\mathrm{p})_\beta + \varepsilon_\sigma(\rho c_\mathrm{p})_\sigma. \tag{11}$$

3.2. *Average equations*

Applying the volume average method to Eqs. (1) and (2) in the case of a homogeneous medium for the β-phase, we get

$$\begin{aligned}&(\rho c_\mathrm{p})_\beta\left(\varepsilon_\beta\frac{\partial\langle T_\beta\rangle^\beta}{\partial t}\nabla\cdot\langle T_\beta\vec{v}_\beta\rangle\right) = \nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle T_\beta\rangle^\beta\right)\\ &\quad+\nabla\cdot\left[k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}T_\beta\,\mathrm{d}A\right)\right]\\ &\quad+k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\alpha}\cdot\nabla T_\beta\,\mathrm{d}A\right)\end{aligned} \tag{12}$$

and, for the σ-phase

$$\begin{aligned}&(\rho c_\mathrm{p})_\sigma\varepsilon_\sigma\frac{\partial\langle T_\sigma\rangle^\sigma}{\partial t} = \nabla\cdot\left(\varepsilon_\sigma k_\sigma\nabla\langle T_\sigma\rangle^\sigma\right)\\ &\quad+\nabla\cdot\left[k_\sigma\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\sigma\beta}T_\sigma\,\mathrm{d}A\right)\right]\\ &\quad+k_\sigma\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\sigma\beta}\cdot\nabla T_\sigma\,\mathrm{d}A\right).\end{aligned} \tag{13}$$

Let us now introduce the following decomposition for the local velocity

$$\vec{v}_\beta = \langle\vec{v}_\beta\rangle^\beta + \tilde{\vec{v}}_\beta \tag{14}$$

Using this equation in Eq. (12), we get

$$\begin{aligned}
&\varepsilon_\beta(\rho c_\mathrm{p})_\beta\left(\frac{\partial\langle T_\beta\rangle^\beta}{\partial t}+\langle\vec{v}\rangle^\beta\cdot\nabla\langle T_\beta\rangle^\beta+\nabla\cdot\langle T_\beta\tilde{\vec{v}}_\beta\rangle^\beta\right)\\
&\quad=\nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle T_\beta\rangle^\beta\right)\\
&\qquad+\nabla\cdot\left[k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}T_\beta\,\mathrm{d}A\right)\right]\\
&\qquad+k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\cdot\nabla T_\beta\,\mathrm{d}A\right).
\end{aligned}\tag{15}$$

Here, we have used the fact that $\langle\langle\vec{v}_\beta\rangle^\beta\rangle^\beta=\langle\vec{v}_\beta\rangle^\beta$ and also the fact that, due to the adherence condition for the fluid in the $A_{\beta\sigma}$ interface:

$$\langle\nabla\cdot\vec{v}_\beta\rangle=\nabla\cdot\langle\vec{v}_\beta\rangle+\frac{1}{V}\int_{A_{\beta\sigma}}\vec{v}_\beta\cdot\vec{n}_{\beta\sigma}\,\mathrm{d}A=\varepsilon_\beta\nabla\cdot\langle\vec{v}_\beta\rangle^\beta=0.$$

In addition, let us define the pore-scale deviations for the β-phase and the σ-phase as

$$T_\beta=\langle T\rangle+\tilde{T}_\beta,\tag{16}$$

$$T_\sigma=\langle T\rangle+\tilde{T}_\sigma,\tag{17}$$

where $\langle T\rangle$ represents the spatial average temperature of the medium. If we replace these deviations in Eq. (10), we get the following constraint for the spatial deviation temperatures

$$\varepsilon_\beta(\rho c_\mathrm{p})_\beta\langle\tilde{T}_\beta\rangle^\beta+\varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\langle\tilde{T}_\sigma\rangle^\sigma=0.\tag{18}$$

One can now introduce the first decomposition (16) in Eq. (15) to obtain

$$\begin{aligned}
&\varepsilon_\beta(\rho c_\mathrm{p})_\beta\left(\frac{\partial\langle T\rangle}{\partial t}+\langle\vec{v}_\beta\rangle^\beta\cdot\nabla\langle T\rangle\right)\\
&\quad=\nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle T\rangle\right)+\nabla\cdot\left[k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\langle T\rangle\,\mathrm{d}A\right)\right]\\
&\qquad+k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\cdot\nabla\langle T\rangle\,\mathrm{d}A\right)\\
&\qquad+\nabla\cdot\left[k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_\beta\tilde{T}_\beta\,\mathrm{d}A\right)\right]\\
&\qquad+k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\cdot\nabla\tilde{T}_\beta\,\mathrm{d}A\right)\\
&\qquad-\varepsilon_\beta(\rho c_\mathrm{p})_\beta\left(\langle\vec{v}_\beta\rangle^\beta\cdot\nabla\langle\tilde{T}_\beta\rangle^\beta+\nabla\cdot\langle\tilde{T}_\beta\tilde{\vec{v}}_\beta\rangle^\beta\right)\\
&\qquad-\varepsilon_\beta(\rho c_\mathrm{p})_\beta\frac{\partial\langle\tilde{T}_\beta\rangle^\beta}{\partial t}+\nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle\tilde{T}_\beta\rangle^\beta\right).
\end{aligned}\tag{19}$$

Here, we have assumed that, as a first approximation, $\langle\tilde{\vec{v}}_\beta\rangle=0$; but we do not consider that $\langle\tilde{T}_\beta\rangle^\beta=\langle\tilde{T}_\beta\rangle^\sigma=0$.

Since $\langle T\rangle$ and $\nabla\langle T\rangle$ can be considered constant with respect to integration over $A_{\beta\sigma}$ [2], they can be removed from the integrals and the volume average theorem can be applied to yield

$$\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\langle T\rangle\,\mathrm{d}A=\langle T\rangle\left(\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\,\mathrm{d}A\right)=-\langle T\rangle\nabla\varepsilon_\beta=0,$$

$$\begin{aligned}
&\int_{A_{\beta\sigma}}\vec{n}_{\beta\alpha}\cdot\nabla\langle T\rangle\,\mathrm{d}A=\nabla\langle T\rangle\cdot\left(\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\,\mathrm{d}A\right)\\
&\quad=-\nabla\langle T\rangle\cdot\nabla\varepsilon_\beta=0.
\end{aligned}$$

Then we can write

$$\begin{aligned}
&\varepsilon_\beta(\rho c_\mathrm{p})_\beta\left(\frac{\partial\langle T\rangle}{\partial t}+\langle\vec{v}_\beta\rangle^\beta\cdot\nabla\langle T\rangle\right)\\
&\quad=\nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle T\rangle\right)+\nabla\cdot\left[k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\tilde{T}_\beta\,\mathrm{d}A\right)\right]\\
&\qquad+k_\beta\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\beta\sigma}\cdot\nabla\tilde{T}_\beta\,\mathrm{d}A\right)\\
&\qquad-\varepsilon_\beta(\rho c_\mathrm{p})_\beta\nabla\cdot\langle\tilde{T}_\beta\tilde{\vec{v}}_\beta\rangle^\beta-\varepsilon_\beta(\rho c_\mathrm{p})_\beta\frac{\partial\langle\tilde{T}_\beta\rangle^\beta}{\partial t}\\
&\qquad+\nabla\cdot\left(\varepsilon_\beta k_\beta\nabla\langle\tilde{T}_\beta\rangle^\beta\right).
\end{aligned}\tag{20}$$

A similar procedure can be followed to obtain the analogous form for the σ-phase

$$\begin{aligned}
&\varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\frac{\partial\langle T\rangle}{\partial t}\\
&\quad=\nabla\cdot\left(\varepsilon_\sigma k_\sigma\nabla\langle T\rangle\right)+\nabla\cdot\left[k_\sigma\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\sigma\beta}\tilde{T}_\sigma\,\mathrm{d}A\right)\right]\\
&\qquad+k_\sigma\left(\frac{1}{V}\int_{A_{\beta\sigma}}\vec{n}_{\sigma\beta}\cdot\nabla\tilde{T}_\sigma\,\mathrm{d}A\right)\\
&\qquad-\varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\frac{\partial\langle\tilde{T}_\sigma\rangle^\sigma}{\partial t}+\nabla\cdot\left(\varepsilon_\sigma k_\sigma\nabla\langle\tilde{T}_\sigma\rangle^\sigma\right).
\end{aligned}\tag{21}$$

Eqs. (20) and (21) can now be added to obtain a single equation

$$
\begin{aligned}
&\langle \rho c_{\mathrm{p}}\rangle \frac{\partial \langle T\rangle}{\partial t} + \varepsilon_\beta (\rho c_{\mathrm{p}})_\beta \langle \vec{v}_\beta\rangle^\beta \cdot \nabla \langle T\rangle \\
&\quad = \nabla \cdot \Bigg[\big(\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma\big) \nabla \langle T\rangle \\
&\qquad + \frac{\big(k_\beta - k_\sigma\big)}{V} \int_{A_{\beta\sigma}} \vec{n}_{\beta\sigma} \tilde{T}_\beta \, \mathrm{d}A \Bigg] - \varepsilon_\beta (\rho c_{\mathrm{p}})_\beta \nabla \cdot \langle \tilde{T}_\beta \vec{v}_\beta\rangle^\beta \\
&\qquad + \nabla \cdot \Big(\varepsilon_\beta k_\beta \nabla \langle \tilde{T}_\beta\rangle^\beta + \varepsilon_\sigma k_\sigma \nabla \langle \tilde{T}_\sigma\rangle^\sigma \Big)
\end{aligned}
\tag{22}
$$

where we have taken into account the boundary conditions (3) and (4).

3.3. Closure problem

To derive a governing equation for $\tilde{T}_\beta$, we begin by using the decomposition equation (16) in the microscopic equation (1) for the β-phase

$$
\begin{aligned}
&(\rho c_{\mathrm{p}})_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \tilde{T}_\beta - \nabla \cdot \Big(k_\beta \nabla \tilde{T}_\beta \Big) \\
&\quad = -(\rho c_{\mathrm{p}})_\beta \frac{\partial \langle T\rangle}{\partial t} - (\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \langle T\rangle + \nabla \cdot \big(k_\beta \nabla \langle T\rangle \big)
\end{aligned}
\tag{23}
$$

and the pore-scale boundary conditions become

$$
\tilde{T}_\beta = \tilde{T}_\sigma \quad \text{at } A_{\beta\sigma} \tag{24}
$$

$$
\begin{aligned}
&\vec{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta = \vec{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma + \vec{n}_{\beta\sigma} \cdot \big(k_\sigma - k_\beta\big) \nabla \langle T\rangle \\
&\quad \text{at } A_{\beta\sigma}
\end{aligned}
\tag{25}
$$

In this study, we shall consider that the time scales associated with the pore-scale equations are much smaller than the time associated (t^*) with the average equations

$$
\frac{(\rho c_{\mathrm{p}})_\beta}{k_\beta} \frac{\ell_\beta^2}{t^*} \ll 1
$$

and

$$
\frac{(\rho c_{\mathrm{p}})_\beta}{k_\sigma} \frac{\ell_\beta^2}{t^*} \ll 1,
$$

where ℓ_β and ℓ_σ are the length scales associated with the pore size ($\sim \ell$). This allows us to consider the closure problems as quasi-steady

$$
\begin{aligned}
&(\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \tilde{T}_\beta - \nabla \cdot \Big(k_\beta \nabla \tilde{T}_\beta \Big) \\
&\quad = -(\rho c_{\mathrm{p}})_\beta \frac{\partial \langle T\rangle}{\partial t} - (\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \langle T\rangle + \nabla \cdot \big(k_\beta \nabla \langle T\rangle \big).
\end{aligned}
\tag{26}
$$

Now using the average equation (22) to express the term $\partial\langle T\rangle/\partial t$,

$$
\begin{aligned}
&(\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \tilde{T}_\beta \\
&\quad = \nabla \cdot \Big(k_\beta \nabla \tilde{T}_\beta \Big) + \frac{(\rho c_{\mathrm{p}})_\beta}{\langle \rho c_{\mathrm{p}}\rangle} \Bigg\{ \varepsilon_\beta (\rho c_{\mathrm{p}})_\beta \langle \vec{v}_\beta\rangle^\beta \cdot \nabla \langle T\rangle \\
&\qquad - \nabla \cdot \Bigg[\big(\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma\big) \nabla \langle T\rangle \\
&\qquad + \frac{\big(k_\beta - k_\sigma\big)}{V} \int_{A_{\beta\sigma}} \vec{n}_{\beta\sigma} \tilde{T}_\beta \, \mathrm{d}A + \varepsilon_\beta k_\beta \nabla \langle \tilde{T}_\beta\rangle^\beta \\
&\qquad + \varepsilon_\sigma k_\sigma \nabla \langle \tilde{T}_\sigma\rangle^\sigma \Bigg] - \varepsilon_\beta (\rho c_{\mathrm{p}})_\beta \nabla \cdot \langle \tilde{T}_\beta \vec{v}_\beta\rangle^\beta \Bigg\} \\
&\qquad - (\rho c_{\mathrm{p}})_\beta \vec{v}_\beta \cdot \nabla \langle T\rangle + \nabla \cdot \big(k_\beta \nabla \langle T\rangle \big).
\end{aligned}
\tag{27}
$$

From the pore-scale boundary condition (25) we can estimate the order of magnitude of the deviations as

$$
\tilde{T}_{\beta,\,\sigma} = \mathcal{O}\left(\frac{\ell_{\beta,\,\sigma} \langle T\rangle}{L} \right), \tag{28}
$$

where L is the distance over which significant variations in the averaged quantities occur. The analysis of the order of magnitude of the different terms in Eq. (27) [2] shows that,

$$
\vec{v}_\beta \cdot \nabla \tilde{T}_\beta = \mathcal{O}\left(\frac{v_\beta \tilde{T}_\beta}{\ell_\beta} \right), \tag{29}
$$

$$
\varepsilon_\beta \langle \vec{v}_\beta\rangle \cdot \nabla \langle T\rangle = \mathcal{O}\left(\frac{\langle v_\beta\rangle^\beta \tilde{T}_\beta}{\ell_\beta} \right), \tag{30}
$$

$$
\vec{v}_\beta \cdot \nabla \langle T\rangle = \mathcal{O}\left(\frac{v_\beta \tilde{T}_\beta}{\ell_\beta} \right), \tag{31}
$$

$$
\varepsilon_\beta \nabla \cdot \langle \vec{v}_\beta \tilde{T}_\beta\rangle^\beta = \mathcal{O}\left(\frac{\langle v_\beta\rangle^\beta \tilde{T}_\beta}{L} \right). \tag{32}
$$

Since the constraint on the length scales requires that $\ell_{\beta,\,\sigma} \ll L$, the last term can be dropped relative to the other three terms. Furthermore, from the other terms

$$
\nabla \cdot \Big(k_\beta \nabla \tilde{T}_\beta \Big) = \mathcal{O}\left(\frac{k_\beta \tilde{T}_\beta}{\ell_\beta^2} \right), \tag{33}
$$

$$
\nabla \cdot \big(\varepsilon_{\beta,\,\sigma}\, k_{\beta,\,\sigma} \nabla \langle T\rangle \big) = \mathcal{O}\left(\frac{k_{\beta,\,\sigma} \tilde{T}_{\beta,\,\sigma}}{\ell_{\beta,\,\sigma} L} \right), \tag{34}
$$

$$\nabla \cdot \left[\frac{(k_\beta - k_\sigma)}{V} \int_{A_{\beta\sigma}} \vec{n}_{\beta\sigma} \tilde{T}_\beta \, \mathrm{d}A \right] = \mathcal{O}\left(\frac{k \tilde{T}_\beta}{\ell L} \right), \tag{35}$$

$$\nabla \cdot \left(k_\beta \nabla \langle T \rangle \right) = \mathcal{O}\left(\frac{k_\beta \tilde{T}_\beta}{\ell_\beta L} \right), \tag{36}$$

$$\nabla \cdot \left(\varepsilon_{\beta,\sigma} k_{\beta,\sigma} \nabla \langle \tilde{T}_{\beta,\sigma} \rangle^{\beta,\sigma} \right) = \mathcal{O}\left(\frac{k_{\beta,\sigma} \langle \tilde{T}_{\beta,\sigma} \rangle^{\beta,\sigma}}{L^2} \right), \tag{37}$$

and the last four terms can be neglected with respect to the first. Therefore, removing these terms, the equations and boundary conditions for the temperature deviations become

$$\begin{aligned} &(\rho c_\mathrm{p})_\beta \vec{v}_\beta \cdot \nabla \tilde{T}_\beta \\ &\quad = \nabla \cdot \left(k_\beta \nabla \tilde{T}_\beta \right) - (\rho c_\mathrm{p})_\beta \left[\vec{v}_\beta - \frac{\varepsilon_\beta (\rho c_\mathrm{p})_\beta}{\langle \rho c_\mathrm{p} \rangle} \langle \vec{v}_\beta \rangle^\beta \right] \\ &\qquad \cdot \nabla \langle T \rangle \end{aligned} \tag{38}$$

$$\tilde{T}_\beta = \tilde{T}_\sigma \quad \text{at } A_{\beta\sigma} \tag{39}$$

$$\vec{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta = \vec{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma + \vec{n}_{\beta\sigma} \cdot \left(k_\sigma - k_\beta \right) \nabla \langle T \rangle \quad \text{at } A_{\beta\sigma} \tag{40}$$

The same can be done for the σ-phase to obtain

$$0 = \nabla \cdot \left(k_\sigma \nabla \tilde{T}_\sigma \right) + (\rho c_\mathrm{p})_\sigma \left[\frac{\varepsilon_\beta (\rho c_\mathrm{p})_\beta}{\langle \rho c_\mathrm{p} \rangle} \right] \langle \vec{v}_\beta \rangle^\beta \cdot \nabla \langle T \rangle. \tag{41}$$

There are some macroscopic source terms involving $\nabla \langle T \rangle$ in these equations. So a closed form of the Eq. (22) can be obtained if the deviations are represented in terms of these macroscopic terms:

$$\tilde{T}_\beta = \vec{f} \cdot \nabla \langle T \rangle \tag{42}$$

$$\tilde{T}_\sigma = \vec{g} \cdot \nabla \langle T \rangle \tag{43}$$

We now introduce the deviation representations (42) and (43) in the deviation equations (38) and (41) to obtain

$$\begin{aligned} &(\rho c_\mathrm{p})_\beta \vec{v}_\beta \cdot \left(\nabla \vec{f} \right) \\ &\quad = \nabla \left(k_\beta \nabla \vec{f} \right) - (\rho c_\mathrm{p})_\beta \left[\vec{v}_\beta - \frac{\varepsilon_\beta (\rho c_\mathrm{p})_\beta}{\langle \rho c_\mathrm{p} \rangle} \langle \vec{v}_\beta \rangle^\beta \right] \end{aligned} \tag{44}$$

$$0 = \nabla \cdot \left(k_\sigma \nabla \vec{g} \right) + (\rho c_\mathrm{p})_\sigma \left[\frac{\varepsilon_\beta (\rho c_\mathrm{p})_\beta}{\langle \rho c_\mathrm{p} \rangle} \right] \langle \vec{v}_\beta \rangle^\beta \tag{45}$$

$$\vec{f} = \vec{g} \quad \text{at } A_{\beta\sigma} \tag{46}$$

$$k_\beta \, \vec{n}_{\beta\sigma} \cdot \left(\nabla \vec{f} \right) = k_\sigma \, \vec{n}_{\beta\sigma} \cdot \left(\nabla \vec{g} \right) + \left(k_\sigma - k_\beta \right) \vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma} \tag{47}$$

Introducing these representations in Eq. (22) gives the macroscopic equations for the one-equation model:

$$\begin{aligned} &\langle \rho c_\mathrm{p} \rangle \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_\mathrm{p})_\beta \langle \vec{v}_\beta \rangle^\beta \cdot \nabla \langle T \rangle \\ &\quad = \nabla \cdot \left(\overline{\overline{K}}_\mathrm{eff} \nabla \langle T \rangle \right). \end{aligned} \tag{48}$$

In this equation, the effective thermal dispersion tensor is given by

$$\begin{aligned} \overline{\overline{K}}_\mathrm{eff} = {} & \left(\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma \right) \overline{\overline{I}} + \varepsilon_\beta k_\beta \overline{\overline{\tau}}_\beta + \varepsilon_\sigma k_\sigma \overline{\overline{\tau}}_\sigma \\ & - \varepsilon_\beta (\rho c_\mathrm{p})_\beta \overline{\overline{D}}, \end{aligned} \tag{49}$$

and the second-order tensors $\overline{\overline{\tau}}_{\beta,\sigma}$ and $\overline{\overline{D}}$ by

$$\overline{\overline{\tau}}_{\beta,\sigma} = \frac{1}{V_{\beta,\sigma}} \int_{A_{\beta\sigma}} \vec{n}_{\beta\sigma,\sigma\beta} \vec{f} \, \mathrm{d}A \tag{50}$$

$$\overline{\overline{D}} = \frac{1}{V_\beta} \int_{V_\beta} \vec{v}_\beta \vec{f} \, \mathrm{d}V \tag{51}$$

In obtaining Eq. (48) the last two *third-order* terms in $\langle T \rangle$ in Eq. (22) have been neglected.

The solutions to the two closure problems (44) and (45), the vectors $\vec{f}$ and $\vec{g}$, can be obtained within about a same constant. Nevertheless, this constant is very important for evaluating the effective thermal dispersion tensor. This indetermination has to be removed using Eqs. (42) and (43) in Eq. (18)

$$0 = \left[\varepsilon_\beta (\rho c_\mathrm{p})_\beta \langle \vec{f} \rangle^\beta + \varepsilon_\sigma (\rho c_\mathrm{p})_\sigma \langle \vec{g} \rangle^\sigma \right] \cdot \nabla \langle T \rangle \tag{52}$$

and therefore

$$\varepsilon_\beta (\rho c_\mathrm{p})_\beta \langle \vec{f} \rangle^\beta + \varepsilon_\sigma (\rho c_\mathrm{p})_\sigma \langle \vec{g} \rangle^\sigma = 0. \tag{53}$$

An important point must be emphasized here. This new closure does not require *an absolute* local thermal equilibrium, i.e. $\langle \vec{f} \rangle^\beta = \langle \vec{g} \rangle^\sigma = 0$. Moreover, the *exact* value of the disequilibrium, i.e. the values of $\langle \vec{f} \rangle^\beta$ or $\langle \vec{g} \rangle^\sigma$ related by Eq. (53), play a role in determining the thermal dispersion tensor.

Now as a demonstration of the exactitude of the above approach, we will prove it using the classical homogenization technique.

4. Homogenization method

As we already know, two length scales are associated with this problem: the macroscopic length L associated with the dimension of the porous medium, i.e. the distance over which significant variations in the averaged temperature occur; and the microscopic characteristic length ℓ associated with the pore size, which is of the same order of magnitude as the periodic cell dimension. The mathematical procedure employed here is a multiple scale expansion [3], and we shall apply it to up-scale the thermal dispersion in the porous medium. The procedure developed here is similar to that one employed by Bloch and Auriault [6] for heat transfer in non-saturated porous media. For this purpose, two independent coordinate systems are introduced, x for the macroscopic scale and y for the microscopic scale. This assumes that the ratio $\varepsilon = \ell/L$ is small.

Let us now introduce the dimensionless form of Eqs. (1)–(4)

$$\frac{\partial T_\beta}{\partial t^*} + Pe\,\vec{v}^*_\beta \cdot \nabla^* T_\beta = \nabla^{*2} T_\beta \tag{54}$$

$$\frac{\alpha_\beta}{\alpha_\sigma}\frac{\partial T_\sigma}{\partial t^*} = \nabla^{*2} T_\sigma \tag{55}$$

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \tag{56}$$

$$\frac{k_\beta}{k_\sigma}\left(\nabla^* T_\beta\right) \cdot \vec{n}_{\beta\sigma} = \left(\nabla^* T_\sigma\right) \cdot \vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma} \tag{57}$$

Here, $t^* = \alpha_\beta t/\ell^2$, $Pe = v_{\text{ref}}\ell/\alpha_\beta$ is the Péclet number, $\vec{v}^*_\beta = \vec{v}_\beta/v_{\text{ref}}$ where v_{ref} is a reference velocity characteristic of the average fluid velocity, and $\nabla^* = \ell\nabla$. In the following, we shall consider that the ratios of heat conductivity (k_β/k_σ) and thermal diffusivity $(\alpha_\beta/\alpha_\sigma)$ are of the order of magnitude $\mathcal{O}(1)$.

Due to the separation of scales, we define two dimensionless variables $x^* = x/L$ and $y^* = y/\ell$ associated with the macroscopic scale L and with the microscopic scale, respectively. Since the two space variables x and y are independent,

$$\begin{aligned}\nabla^* &= \ell\nabla = \ell\left(\nabla_x + \nabla_y\right) = \ell\left(\frac{1}{L}\nabla^*_x + \frac{1}{\ell}\nabla^*_y\right)\\ &= \epsilon\nabla^*_x + \nabla^*_y.\end{aligned} \tag{58}$$

We also consider here that two time scales are associated with the thermal dispersion macroscopic problem at the macroscopic scale: one time scale characteristic for convection (L/v_{ref}) and another for diffusion (L^2/α_β). Thus, %

$$t^*_{\text{c}} = \frac{v_{\text{ref}}t}{L} \quad \text{and} \quad t^*_{\text{d}} = \frac{\alpha_\beta t}{L^2} \tag{59}$$

leads to

$$\frac{\partial}{\partial t^*} = \varepsilon Pe\frac{\partial}{\partial t^*_{\text{c}}} + \epsilon^2\frac{\partial}{\partial t^*_{\text{d}}}, \tag{60}$$

and we must look for $T(x^*, y^*, t^*_{\text{c}}, t^*_{\text{d}})$ verifying

$$\begin{aligned}&\varepsilon Pe\frac{\partial T_\beta}{\partial t^*_{\text{c}}} + \epsilon^2\frac{\partial T_\beta}{\partial t^*_{\text{d}}} + Pe\,\vec{v}^*_\beta \cdot \left(\nabla^*_y T_\beta + \epsilon\nabla^*_x T_\beta\right)\\ &\quad = \left(\nabla^*_y + \epsilon\nabla^*_x\right) \cdot \left(\nabla^*_y T_\beta + \epsilon\nabla^*_x T_\beta\right)\end{aligned} \tag{61}$$

$$\begin{aligned}&\frac{\alpha_\beta}{\alpha_\sigma}\left(\epsilon Pe\frac{\partial T_\sigma}{\partial t^*_{\text{c}}} + \epsilon^2\frac{\partial T_\sigma}{\partial t^*_{\text{d}}}\right)\\ &\quad = \left(\nabla^*_y + \epsilon\nabla^*_x\right) \cdot \left(\nabla^*_y T_\sigma + \epsilon\nabla^*_x T_\sigma\right)\end{aligned} \tag{62}$$

and

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \tag{63}$$

$$\begin{aligned}&\frac{k_\beta}{k_\sigma}\left(\nabla^*_y T_\beta + \epsilon\nabla^*_x T_\beta\right) \cdot \vec{n}_{\beta\sigma} = \left(\nabla^*_y T_\sigma + \epsilon\nabla^*_x T_\sigma\right) \cdot \vec{n}_{\beta\sigma}\\ &\quad \text{at } A_{\beta\sigma}\end{aligned} \tag{64}$$

Different results may be obtained depending on the order of magnitude of the Péclet number Pe [3]. For $Pe = \mathcal{O}(\varepsilon^n)$ with $n \geq 2$, the homogenized equation is a conductive equation with the equivalent classical conductivity of the diffusion problem for a two-phase system. For $Pe = O(\varepsilon)$, to the preceding equation a convective term corresponding to the average movement of the fluid (β) phase must be added. For $Pe = \mathcal{O}(\varepsilon^n)$ with $n \leq -1$, the multiple scale method is unable to provide a homogenized behavior. The most interesting situation is $Pe = \mathcal{O}(\varepsilon^0)$.

It can be easier to work with *dimensional* variables, with the recalling the order of magnitude of the different terms. Hence,

$$\begin{aligned}&\epsilon\frac{\partial T_\beta}{\partial t_{\text{c}}} + \epsilon^2\frac{\partial T_\beta}{\partial t_{\text{d}}} + \vec{v}_\beta \cdot \left(\nabla_y T_\beta + \epsilon\nabla_x T_\beta\right)\\ &\quad = \left(\nabla_y + \epsilon\nabla_x\right) \cdot \left[\alpha_\beta\left(\nabla_y T_\beta + \epsilon\nabla_x T_\beta\right)\right]\end{aligned} \tag{65}$$

$$\epsilon\frac{\partial T_\sigma}{\partial t_{\mathrm{c}}}+\epsilon^2\frac{\partial T_\sigma}{\partial t_{\mathrm{d}}} = (\nabla_y+\epsilon\nabla_x)\cdot\left[\alpha_\sigma(\nabla_y T_\sigma+\epsilon\nabla_x T_\sigma)\right] \tag{66}$$

and

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \tag{67}$$

$$k_\beta(\nabla_y T_\beta+\epsilon\nabla_x T_\beta)\cdot\vec{n}_{\beta\sigma} = k_\sigma(\nabla_y T_\sigma+\epsilon\nabla_x T_\sigma)\cdot\vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma} \tag{68}$$

The spatially periodic velocity field $\vec{v}_\beta$ is dependent only on the y variable, and is divergence-free (incompressible fluid)

$$\nabla_y\cdot\vec{v}_\beta = 0. \tag{69}$$

Here, it is assumed that the temperatures can be expanded in the form of an asymptotic expansion in ε

$$T_\beta(x,y,t_{\mathrm{c}},t_{\mathrm{d}}) = \sum_{k=0}^{k=\infty}\epsilon^k T_\beta^k(x,y,t_{\mathrm{c}},t_{\mathrm{d}}), \tag{70}$$

$$T_\sigma(x,y,t_{\mathrm{c}},t_{\mathrm{d}}) = \sum_{k=0}^{k=\infty}\epsilon^k T_\sigma^k(x,y,t_{\mathrm{c}},t_{\mathrm{d}}), \tag{71}$$

At the order ϵ^0, T_β^0 and T_σ^0 should satisfy

$$\vec{v}_\beta\cdot\nabla_y T_\beta^0 = \nabla_y\cdot\left(\alpha_\beta\nabla_y T_\beta^0\right) \tag{72}$$

$$0 = \nabla_y\cdot\left(\alpha_\sigma\nabla_y T_\sigma^0\right) \tag{73}$$

and

$$T_\beta^0 = T_\sigma^0 \quad \text{at } A_{\beta\sigma} \tag{74}$$

$$k_\beta\left(\nabla_y T_\beta^0\right)\cdot\vec{n}_{\beta\sigma} = k_\sigma\left(\nabla_y T_\sigma^0\right)\cdot\vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma} \tag{75}$$

along with periodic boundary conditions at the edge of the unit cell. The solution to the above problem is satisfied by

$$T_\beta^0(x,y,t_{\mathrm{c}},t_{\mathrm{d}}) = T_\sigma^0(x,y,t_{\mathrm{c}},t_{\mathrm{d}}) = T^0(x,t_{\mathrm{c}},t_{\mathrm{d}}). \tag{76}$$

From the work of Auriault and Lewandowska [7] this condition, Eq. (76), means that a *relative* local equilibrium is met as a first-order approximation of the temperature. The authors consider that there exists a local non-equilibrium if this result is not obtained.

The next order, ϵ^1, yields

$$\frac{\partial T^0}{\partial t_{\mathrm{c}}}+\vec{v}_\beta\cdot\left(\nabla_y T_\beta^1+\nabla_x T^0\right) = \nabla_y\cdot\left[\alpha_\beta\left(\nabla_y T_\beta^1+\nabla_x T^0\right)\right] \tag{77}$$

$$\frac{\partial T^0}{\partial t_{\mathrm{c}}} = \nabla_y\cdot\left[\alpha_\sigma\left(\nabla_y T_\sigma^1+\nabla_x T^0\right)\right] \tag{78}$$

and

$$T_\beta^1 = T_\sigma^1 \quad \text{at } A_{\beta\sigma} \tag{79}$$

$$k_\beta\left(\nabla_y T_\beta^1+\nabla_x T^0\right)\cdot\vec{n}_{\beta\sigma} = k_\sigma\left(\nabla_y T_\sigma^1+\nabla_x T^0\right)\cdot\vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma} \tag{80}$$

with periodic boundary conditions in y at the unit cell boundaries.Taking the volume average over the unit cell ($V = V_\beta\cup V_\sigma$) of Eqs. (77) and (78) and adding the results leads to

$$\langle\rho c_{\mathrm{p}}\rangle\frac{\partial T^0}{\partial t_{\mathrm{c}}}+\frac{1}{V}\int_{V_\beta}(\rho c_{\mathrm{p}})_\beta\vec{v}_\beta\cdot\left(\nabla_y T_\beta^1+\nabla_x T^0\right)\mathrm{d}V = 0, \tag{81}$$

where $\langle\rho c_{\mathrm{p}}\rangle = \varepsilon_\beta(\rho c_{\mathrm{p}})_\beta+\varepsilon_\sigma(\rho c_{\mathrm{p}})_\sigma$ is the average heat capacity per unit volume of the medium.

As $\vec{v}_\beta\cdot\nabla_y T_\beta^1 = \nabla_y\cdot(\vec{v}_\beta T_\beta^1)$ and $\vec{v}_\beta$ and T_β^1 are spatially y-periodic, with the no-slip condition on $A_{\beta\sigma}$

$$\langle\rho c_{\mathrm{p}}\rangle\frac{\partial T^0}{\partial t_{\mathrm{c}}}+\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{v}_\beta\rangle^\beta\cdot\nabla_x T^0 = 0 \tag{82}$$

and we see that at the first order the transport at the macroscopic scale is only convective.

Using this equation to replace the transient terms in Eqs. (77) and (78), we obtain

$$(\rho c_{\mathrm{p}})_\beta\vec{v}_\beta\cdot\nabla_y T_\beta^1 = \nabla_y\cdot\left(k_\beta\nabla_y T_\beta^1\right)-(\rho c_{\mathrm{p}})_\beta\left[\vec{v}_\beta-\frac{\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta}{\langle\rho c_{\mathrm{p}}\rangle}\langle\vec{v}_\beta\rangle^\beta\right]\cdot\nabla_x T^0 \tag{83}$$

and

$$0 = \nabla_y\cdot\left(k_\sigma\nabla_y T_\sigma^1\right)+(\rho c_{\mathrm{p}})_\sigma\left[\frac{\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta}{\langle\rho c_{\mathrm{p}}\rangle}\right]\langle\vec{v}_\beta\rangle^\beta\cdot\nabla_x T^0 \tag{84}$$

with the appropriate boundary conditions given by Eqs. (79) and (80).

This problem, Eqs. (83) and (84), is similar to the one encountered in Section 3.3, and we propose the solution in the form

$$T_\beta^1 = \vec{f}(y) \cdot \nabla_x T^0(x, t_c, t_d) + \bar{T}^1(x, t_c, t_d), \tag{85}$$

$$T_\beta^1 = \vec{g}(y) \cdot \nabla_x T^0(x, t_c, t_d) + \bar{T}^1(x, t_c, t_d) \tag{86}$$

where $\vec{f}$ and $\vec{g}$ are solutions of the problems (44)–(47) with periodic boundary conditions over the edges of the unit cell. It is interesting to recall that $\vec{f}$ and $\vec{g}$ are determined within about the same constant and, as we show further on, the determination of this constant is important for the calculation of the thermal dispersion tensor.

Lastly, at order ϵ^2, we have

$$\begin{aligned}\frac{\partial T_\beta^1}{\partial t_c} + \frac{\partial T^0}{\partial t_d} + \vec{v}_\beta \cdot \left(\nabla_y T_\beta^2 + \nabla_x T_\beta^1\right) \\ = \nabla_y \cdot \left[\alpha_\beta\left(\nabla_y T_\beta^2 + \nabla_x T_\beta^1\right)\right] + \nabla_x \cdot \left[\alpha_\beta\left(\nabla_y T_\beta^1 \right.\right. \\ \left.\left. + \nabla_x T^0\right)\right]\end{aligned} \tag{87}$$

$$\begin{aligned}\frac{\partial T_\sigma^1}{\partial t_c} + \frac{\partial T^0}{\partial t_d} = \nabla_y \cdot \left[\alpha_\sigma\left(\nabla_y T_\sigma^2 + \nabla_x T_\sigma^1\right)\right] \\ + \nabla_x\left[\alpha_\sigma\left(\nabla_y T_\sigma^1 + \nabla_x T^0\right)\right]\end{aligned} \tag{88}$$

and

$$T_\beta^2 = T_\sigma^2 \quad \text{at } A_{\beta\sigma} \tag{89}$$

$$\begin{aligned}k_\beta\left(\nabla_x T_\beta^1 + \nabla_y T_\beta^2\right) \cdot \vec{n}_{\beta\sigma} \\ = k_\sigma\left(\nabla_x T_\sigma^1 + \nabla_y T_\sigma^2\right) \cdot \vec{n}_{\beta\sigma} \quad \text{at } A_{\beta\sigma}\end{aligned} \tag{90}$$

In order to find the average equation at order ϵ^2, we take the volume average of Eqs. (87) and (88) and add the results:

$$\begin{aligned}\langle\rho c_p\rangle\left(\frac{\partial\langle T^1\rangle}{\partial t_c} + \frac{\partial T^0}{\partial t_d}\right) + \frac{1}{V}\int_{V_\beta}(\rho c_p)_\beta \vec{v}_\beta \cdot \left(\nabla_y T_\beta^2\right. \\ \left. + \nabla_x T_\beta^1\right) \mathrm{d}V = \frac{1}{V}\int_{V_\beta}\left\{\nabla_y \cdot \left[k_\beta\left(\nabla_y T_\beta^2\right.\right.\right. \\ \left.\left. + \nabla_x T_\beta^1\right)\right] + \nabla_x \cdot \left[k_\beta\left(\nabla_y T_\beta^1 + \nabla_x T^0\right)\right]\Big\} \mathrm{d}V \\ + \frac{1}{V}\int_{V_\sigma}\left\{\nabla_y \cdot \left[k_\sigma\left(\nabla_y T_\sigma^2 + \nabla_x T_\sigma^1\right)\right]\right. \\ \left. + \nabla_x \cdot \left[k_\sigma\left(\nabla_y T_\sigma^1 + \nabla_x T^0\right)\right]\right\} \mathrm{d}V\end{aligned} \tag{91}$$

where

$$\langle\rho c_p\rangle\langle T^1\rangle = \varepsilon_\beta(\rho c_p)_\beta\langle T_\beta^1\rangle^\beta + \varepsilon_\sigma(\rho c_p)_\sigma\langle T_\sigma^1\rangle^\sigma. \tag{92}$$

Using periodic conditions and the no-slip condition over $A_{\beta\sigma}$, it is easy to show that

$$\begin{aligned}\langle\rho c_p\rangle\left(\frac{\partial\langle T^1\rangle}{\partial t_c} + \frac{\partial T^0}{\partial t_d}\right) + \frac{1}{V}\int_{V_\beta}(\rho c_p)_\beta \vec{v}_\beta \cdot \nabla_x T_\beta^1 \,\mathrm{d}V = \\ \frac{1}{V}\int_{V_\beta}\nabla_x \cdot \left[k_\beta\left(\nabla_y T_\beta^1 + \nabla_x T^0\right)\right] \mathrm{d}V \\ + \frac{1}{V}\int_{V_\sigma}\nabla_x \cdot \left[k_\sigma\left(\nabla_y T_\sigma^1 + \nabla_x T^0\right)\right] \mathrm{d}V.\end{aligned} \tag{93}$$

Using (85) in the second term on the left-hand side,

$$\begin{aligned}\frac{1}{V}\int_{V_\beta}(\rho c_p)_\beta \vec{v}_\beta \cdot \nabla_x T_\beta^1 \,\mathrm{d}V \\ = \frac{1}{V}\int_{V_\beta}(\rho c_p)_\beta \nabla_x \cdot \left(T_\beta^1 \vec{v}_\beta\right) \mathrm{d}V \\ = \varepsilon_\beta(\rho c_p)_\beta \nabla_x \cdot \langle T_\beta^1 \vec{v}_\beta\rangle^\beta \\ = \varepsilon_\beta(\rho c_p)_\beta \nabla_x \cdot \left(\langle\vec{v}_\beta \vec{f}\rangle^\beta \cdot \nabla_x T^0 + \bar{T}^1\langle\vec{v}_\beta\rangle^\beta\right)\end{aligned} \tag{94}$$

and, for the other two terms,

$$\begin{aligned}\frac{1}{V}\int_{V_\beta}\nabla_x \cdot \left[k_\beta\left(\nabla_y T_\beta^1 + \nabla_x T^0\right)\right] \mathrm{d}V \\ = \nabla_x \cdot \left\{\left[\varepsilon_\beta k_\beta\left(\langle\nabla_y \vec{f}\rangle^\beta + \bar{\bar{I}}\right)\right] \cdot \nabla_x T^0\right\}\end{aligned} \tag{95}$$

$$\begin{aligned}\frac{1}{V}\int_{V_\sigma}\nabla_x \cdot \left[k_\sigma\left(\nabla_y T_\sigma^1 + \nabla_x T^0\right)\right] \mathrm{d}V \\ = \nabla_x \cdot \left\{\left[\varepsilon_\sigma k_\sigma\left(\langle\nabla_y \vec{g}\rangle^\sigma + \bar{\bar{I}}\right)\right] \cdot \nabla_x T^0\right\}\end{aligned} \tag{96}$$

the average equation at order ϵ^2 is

$$\langle\rho c_{\mathrm{p}}\rangle\left(\frac{\partial\langle T^1\rangle}{\partial t_{\mathrm{c}}}+\frac{\partial T^0}{\partial t_{\mathrm{d}}}\right)$$
$$+\,\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\nabla_x\cdot\left(\langle\vec{v}_\beta\vec{f}\rangle^\beta\cdot\nabla_x T^0+\bar{T}^1\langle\vec{v}_\beta\rangle^\beta\right)$$
$$=\nabla_x\cdot\left\{\left[\left(\varepsilon_\beta k_\beta+\varepsilon_\sigma k_\sigma\right)\bar{\bar{I}}+\varepsilon_\beta k_\beta\langle\nabla_y\vec{f}\rangle^\beta\right.\right.$$
$$\left.\left.+\,\varepsilon_\sigma k_\sigma\langle\nabla_y\vec{g}\rangle^\sigma\right]\cdot\nabla_x T^0\right\}. \tag{97}$$

Lastly, the average transport equation (exact at the order ϵ^2) can be obtained by adding Eqs. (82) and (97):

$$\langle\rho c_{\mathrm{p}}\rangle\left[\epsilon\frac{\partial T^0}{\partial t_{\mathrm{c}}}+\epsilon^2\left(\frac{\partial\langle T^1\rangle}{\partial t_{\mathrm{c}}}+\frac{\partial T^0}{\partial t_{\mathrm{d}}}\right)\right]$$
$$+\,\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{v}_\beta\rangle^\beta\cdot\nabla_x\left(\epsilon T^0+\epsilon^2\bar{T}^1\right)$$
$$=\nabla_x\cdot\left\{\left[\left(\varepsilon_\beta k_\beta+\varepsilon_\sigma k_\sigma\right)\bar{\bar{I}}+\varepsilon_\beta k_\beta\langle\nabla_y\vec{f}\rangle^\beta\right.\right. \tag{98}$$
$$\left.\left.+\,\varepsilon_\sigma k_\sigma\langle\nabla_y\vec{g}\rangle^\sigma\right]\cdot\epsilon^2\nabla_x T^0\right\}$$
$$+\,\nabla_x\cdot\left\{\left[\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{v}_\beta\vec{f}\rangle^\beta\right]\cdot\epsilon^2\nabla_x T^0\right\}.$$

But we know from Eqs. (85), (86) and (92) that

$$\langle T^1\rangle=\frac{1}{\langle\rho c_{\mathrm{p}}\rangle}\left(\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{f}\rangle^\beta+\varepsilon_\sigma(\rho c_{\mathrm{p}})_\sigma\langle\vec{g}\rangle^\beta\right)$$
$$\cdot\nabla_x T^0+\bar{T}^1, \tag{99}$$

and we can remove the unknown constant in the solution to the problem in $\vec{f}$ and $\vec{g}$ by requiring that

$$\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{f}\rangle^\beta+\varepsilon_\sigma(\rho c_{\mathrm{p}})_\sigma\langle\vec{g}\rangle^\beta=0. \tag{100}$$

At order ϵ^2, the average temperature is given by $\langle T\rangle=T^0+\epsilon\langle T^1\rangle=T^0+\epsilon\bar{T}^1$ and the macroscopic equation is given by

$$\langle\rho c_{\mathrm{p}}\rangle\frac{\partial\langle T\rangle}{\partial t}+\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{v}_\beta\rangle^\beta\cdot\nabla\langle T\rangle$$
$$=\nabla\cdot\left(\overline{\overline{K}}_{\mathrm{eff}}\cdot\nabla\langle T\rangle\right)+\mathcal{O}(\epsilon^3), \tag{101}$$

where

$$\overline{\overline{K}}_{\mathrm{eff}}=\left(\varepsilon_\beta k_\beta+\varepsilon_\sigma k_\sigma\right)\bar{\bar{I}}+\varepsilon_\beta k_\beta\langle\nabla_y\vec{f}\rangle^\beta+\varepsilon_\sigma k_\sigma\langle\nabla_y\vec{g}\rangle^\sigma$$
$$-\,\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta\langle\vec{v}_\beta\vec{f}\rangle^\beta. \tag{102}$$

We remark that the two methods (volume average and homogenization) lead to the same macroscopic average equation and closure problems.

5. Results for a stratified medium

Here, we make use of the analytical results for the closure problems for the fully developed flow field between two plates in order to validate and compare with the results of a numerical experiment obtained by the method of random walks. The associated unit cell is represented in Fig. 1, and the flow in the β-phase corresponds to Poiseuille's flow.

For the longitudinal coefficient in our case (see Appendix A) we find

$$K_{xx}=k_\parallel+\varepsilon_\beta^3 Pe^2 k_\beta\left[\frac{17}{140}-\frac{\gamma_\beta}{5}+\frac{\gamma_\beta^2}{12}\right.$$
$$\left.+\,\frac{\gamma_\beta(1-\gamma_\beta)}{12}\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2\right], \tag{103}$$

where $k_\parallel=(\varepsilon_\beta k_\beta+\varepsilon_\sigma k_\sigma)$, Pe is the Péclet number

$$Pe=\frac{\langle u\rangle^\beta H}{\alpha_\beta}=\frac{\langle u\rangle^\beta(h+e)}{\alpha_\beta} \tag{104}$$

and $\gamma_\beta=\varepsilon_\beta(\rho c_{\mathrm{p}})_\beta/\langle\rho c_{\mathrm{p}}\rangle$.

As we have considered in Section 4, $\alpha_\beta/\alpha_\sigma$ is of the order of magnitude $\mathcal{O}(1)$ and Eq. (103) is not valid for $\alpha_\sigma=0$. The only way to obtain a result for $k_\sigma\to0$ is to make $(\rho c_{\mathrm{p}})_\sigma\to0$. In this case, where $\gamma_\beta\to1$ we have the classic expression for the longitudinal coefficient.

5.1. Random walks

In this method, the individual trajectories of convected and diffused *thermions* are calculated. A *ther-*

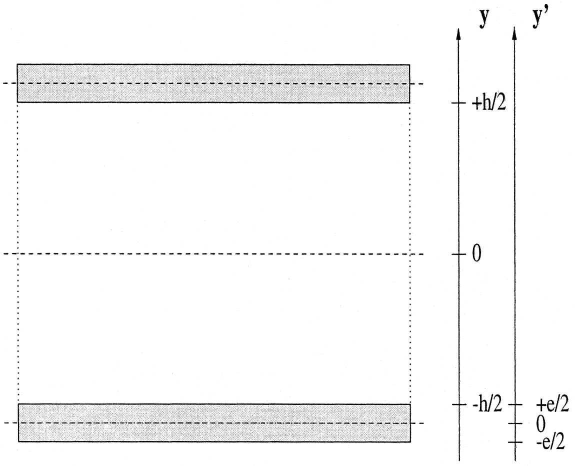

Fig. 1. Unit cell for parallel flow between two planes.

mion is a particle without mass that has a certain quantity of energy (enthalpy), as introduced by Batycky et al. [8] to designate a thermal tracer. The particles are characterized by their positions in space at a given time. Our goal is to calculate the first three moments for the displacement of a large number of *thermions* emanating from a localized source. From the literature (see, for example, [9,10]) we know that the total moment of order zero, M_0, is constant and represents the total quantity of energy released in the medium, that the first moment represents the average position of the *thermions*

$$\vec{M}_1 = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \vec{r}\langle \rho c_{\mathrm{p}}\rangle\langle T\rangle \,\mathrm{d}x\,\mathrm{d}y, \tag{105}$$

and that the second moment describes the spreading of the *thermions*

$$\overline{\overline{M}}_2 = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \vec{r}\vec{r}\langle \rho c_{\mathrm{p}}\rangle\langle T\rangle \,\mathrm{d}x\,\mathrm{d}y. \tag{106}$$

At the limit as time approaches infinity, from Eqs. (48) and (101), the time derivate of the first moment is the mean interstitial fluid velocity multiplied by γ_β

$$\lim_{t\to\infty}\frac{\mathrm{d}\vec{M}_1^*}{\mathrm{d}t} = \lim_{t\to\infty}\frac{1}{M_0}\frac{\mathrm{d}\vec{M}_1}{\mathrm{d}t} = \gamma_\beta\langle\vec{v}_\beta\rangle^\beta \tag{107}$$

and the time derivate of the centered second moment, $\overline{\overline{M}}_2$, is equal to twice the effective thermal dispersion tensor divided by $\langle\rho c_{\mathrm{p}}\rangle$

$$\lim_{t\to\infty}\frac{\mathrm{d}\overline{\overline{M}}_2}{\mathrm{d}t} = \lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\left(\overline{\overline{M}}_2^* - \vec{M}_1^*\vec{M}_1^*\right) = 2\frac{\overline{\overline{K}}_{\mathrm{eff}}}{\langle\rho c_{\mathrm{p}}\rangle}. \tag{108}$$

At time $t = 0$, a large number of *thermions* is released, randomly distributed, at position $x = 0$, which means an impulse of heat equal to $Q\delta_{t=0}\delta_{x=0}$. At each stipulated time step δt the position of each *thermion* is updated by adding a convective displacement and a random diffusive one

$$\vec{r}_i(t+\delta t) = \vec{r}_i(t) + \vec{\delta}_i^{\mathrm{c}} + \delta_i^{\mathrm{d}}, \tag{109}$$

where $\vec{r}_i$ is the vector position of the ith *thermion*, $\delta_i^{\mathrm{c}} = \vec{v}_\beta(\vec{r}_i)\delta t$ is the displacement due to the convection, and $\vec{\delta}_i^{\mathrm{d}}$ due to the diffusion.

The velocity $\vec{v}_\beta(\vec{r}_i)$ is obtained from the analytical solution of the Poiseuille flow

$$u = \langle u\rangle^\beta\left[\frac{3}{2} - 6\left(\frac{y}{h}\right)^2\right]. \tag{110}$$

For the diffusion, we have chosen to make alternate displacements parallel to the x and y axis. This technique consists in moving the *thermion*, for a given time step δt, first to the left or right in the x direction, and then up or down in the y direction in the next time step. At each time, the probability of a move to the left, right, up or down is chosen randomly. The magnitude of the displacements are constant and are given by

$$\delta x_{\beta,\sigma} = \delta y_{\beta,\sigma} = 2\sqrt{\alpha_{\beta,\sigma}\delta t}. \tag{111}$$

The choice of β or σ depends on whether the *thermion* is in the fluid (β-phase) or in the solid (σ-phase).

Whenever a wall collision occurs, a probability of passage into the solid (or fluid) is assigned to the particle. From the results of Appendix B, the probability law of passage into the solid phase is given by

$$p_{\beta\to\sigma} = \frac{b_\sigma}{b_\beta + b_\sigma} \tag{112}$$

and into the fluid phase

$$p_{\sigma\to\beta} = \frac{b_\beta}{b_\beta + b_\sigma} \tag{113}$$

where $b_{\beta,\sigma} = \sqrt{(\rho c_{\mathrm{p}})_{\beta,\sigma}k_{\beta,\sigma}}$. Further, the magnitude of the displacement should change as the particles cross the interface.

When a *thermion* is in a position to cross an interface, it is stopped at the boundary between the β and σ phases before the passage probability is determined. If a randomly chosen number is less than the probability p_σ (or p_β), then the particle will penetrate the solid (or fluid). Otherwise, it makes an elastic rebound.

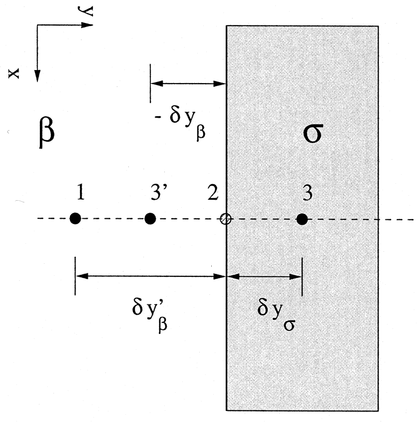

Fig. 2. Wall collision: (1) initial position, (2) at the boundary, (3) passage to the σ-phase and (3′) elastic shock.

Table 1
Thermal conductivity coefficient K_{xx}/k_β for $\varepsilon_\beta = 1$

Theoretical		Numerical		Error%
Pe	K_{xx}/k_β	Pe	K_{xx}/k_β	
1.0	1.01	1.00	0.99	−1.98
5.0	1.12	5.01	1.09	−2.68
10.0	1.48	10.01	1.43	−3.38
50.0	12.91	50.07	12.78	−1.01
100.0	48.62	100.14	48.46	−0.33
500.0	1191.48	500.69	1193.61	+0.18
1000.0	4762.91	1001.38	4774.34	+0.24

But the displacement time must be conserved. So for a particle that has spent a time step $\delta t'_\beta$ to reach at solid wall, a fraction of time $\delta t_{\beta\sigma}$ must be added:

$$\delta t_{\beta\sigma} = \delta t - \delta t'_\beta = \delta t - \frac{\delta y'_\beta 2}{4\alpha_\beta}, \tag{114}$$

where $\delta y'_\beta$ corresponds to the displacement in the time interval $\delta t'_\beta$.

This time will allow the particle to make a displacement equal to

$$\delta y_\sigma = 2\sqrt{\alpha_\sigma \delta t_{\beta\sigma}} \tag{115}$$

if the passage occurs, and

$$\delta y_\beta = -2\sqrt{\alpha_\beta \delta t_{\beta\sigma}} \tag{116}$$

in the case of an elastic shock, as illustrated in Fig. 2.

5.2. Numerical data

The tested cases studied here have been realized for the following physical characteristics: $(\rho c_p)_\beta = 4.0 \times 10^6$ J m^{-3} K^{-1}, $k_\beta = 0.6$ W m^{-1} K^{-1}, $(\rho c_p)_\sigma = 2.0 \times 10^6$ J m^{-3} K^{-1} and $k_\sigma = 1.2$ W m^{-1} K^{-1}. These parameters are approximately consistent with a system of water and glass. For the unity cell we take a unit length and height.

In order to check the exactitude of the numerical results for the random walks method, as very few cases can be solved analytically, we have used the well-known result for the planar Poiseuille flow between two insulated horizontal walls separated by a gap h for the simple case of a stratified medium. For this case, $\varepsilon_\beta = 1$ and the effective longitudinal coefficient is given by

$$\frac{K_{xx}}{k_\beta} = 1 + \frac{Pe^2}{210} \tag{117}$$

All the numerical results have been calculated with 15,000 particles, for a dimensionless time t^* ($t^* = \alpha_\beta t/H^2) = 2$ and for a dimensionless time step $\delta t^* \cong 0.4 \times 10^{-4}$. Here, the Péclet number and the coefficient K_{xx} are both obtained by linear regressions when the linear process is reached for the first moment $\overset{\rightarrow}{\underline{M}}{}_1^*$ and centered second moment $\overline{\overline{M}}_2$ as function of time. In Table 1, we show the results obtained for $\varepsilon_\beta = 1$. As we can see, good agreement is achieved between the theoretical values and the numerical results.

In the Fig. 3, the calculated values of the longitudinal thermal coefficient $K_{xx}/k_\parallel$ are presented for a stratified

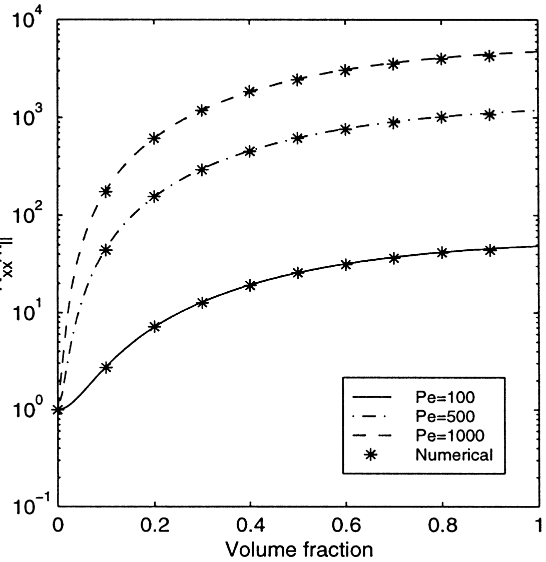

Fig. 3. Longitudinal thermal dispersion coefficient $K_{xx}/k_\parallel$ for a stratified medium.

medium as function of the volume fraction ε_β, and for a dimensionless time approximately equal to 1. These results were obtained for three different values of the Péclet number (100, 500 and 1000) and for the same parameters as those used in the test case, except for the number of particles and dimensionless time step, which are 30,000 and 0.25×10^{-4} here. The numerical results agree quite well with the theoretical prediction of our model for this case. The numerical method of random walks gives the longitudinal coefficients with an error of less than or equal to 3% relative to the theoretical, except for a volume fraction of 0.9, where the error reaches 4.2% for a Péclet number of 1000. This is probably due in part to the small thickness of the solid phase. To overcome this difficulty, a much smaller time step than 0.25×10^{-4} would have to be used, along with a greater number of particles.

In this paper, we are mainly interested in showing the validity of the one-model equation developed here, and the versatility of the random walks method. More sophisticated unit cells can be considered, with a hydrodynamic problem governed by the (Navier–)Stokes equations, and such developments are currently underway to generate numerical data in more complex situations.

6. Conclusion

The thermal dispersion in a spatially periodic porous medium has been investigated using both the method of volume averaging with closure and the method of homogenization in order to obtain a one-equation model. Both methods agree in deriving the same closure problem for calculating the macroscopic effective thermal dispersion tensor $\overline{\overline{K}}_{\text{eff}}$. The important point to be outlined here with the volume averaging approach is that the β-phase and the σ-phase of the medium cannot be in *absolute* thermal equilibrium ($\langle T_\beta\rangle^\beta \neq \langle T_\sigma\rangle^\sigma$) even though a steady-state closure is assumed.

In order to test the validity of the above approach in a simple case (stratified medium), the results of a numerical experiment using the random walks of heat *particles* (*thermions*) are compared with the calculated macroscopic effective thermal dispersion tensor obtained with an analytical solution for the closure problem. Very good agreement is achieved.

This study clearly demonstrates the validity (and also the limitations) of the one-equation model for describing the thermal dispersion process inside a porous medium. The random walk method seems to be a powerful tool to obtain the macroscopic effective thermal dispersion tensor numerically and can be applied in the case of more complex geometries.

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Appendix A

For the one-dimensional unit cell shown in Fig. 1, the closure equations are

$$\frac{d^2 f_x}{dy^2} = \frac{1}{\alpha_\beta}\left(u - \gamma_\beta \langle u\rangle^\beta\right) \tag{A1}$$

and

$$\frac{d^2 g_x}{dy'^{\,2}} = -\frac{1}{\alpha_\sigma}\gamma_\beta \langle u\rangle^\beta \tag{A2}$$

where $\gamma_\beta = \varepsilon_\beta (\rho c_p)_\beta / \langle \rho c_p\rangle$ and $\alpha_{\beta,\,\sigma} = k_{\beta,\,\sigma}/(\rho c_p)_{\beta,\,\sigma}$ are the thermal diffusivity of the β and σ phases.

After integration, we have

$$f_x = \varepsilon_\beta^2\, Pe\, H\left[\left(\frac{3}{4} - \frac{\gamma_\beta}{2}\right)\left(\frac{y}{h}\right)^2 - \frac{1}{2}\left(\frac{y}{h}\right)^4 + A\right] \tag{A3}$$

and

$$g_x = -\varepsilon_\beta^2\, Pe\, H\left[\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2 \frac{\gamma_\beta}{2}\left(\frac{y'}{e}\right)^2 + B\right] \tag{A4}$$

where $Pe = \langle u\rangle^\beta H/\alpha_\beta$ is the Péclet number and $H = h + e$ is the total height of the unit cell.

From the boundary condition at the β–σ interface for $y = -h/2$ for the β-phase and $y' = e/2$ for the σ-phase, we obtain

$$A + B = \frac{\gamma_\beta}{8}\left[1 - \frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2\right] - \frac{5}{32}. \tag{A5}$$

Now if we take the intrinsic volume average of f_x and g_x

$$\langle f\rangle_x^\beta = \varepsilon_\beta^2\, Pe\, H\left(\frac{9}{160} - \frac{\gamma_\beta}{24} + A\right), \tag{A6}$$

$$\langle g_x\rangle^\beta = \varepsilon_\beta^2\, Pe\, H\left[\frac{\gamma_\beta}{24}\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2 + B\right] \tag{A7}$$

and use these results in

$$\varepsilon_\beta(\rho c_\mathrm{p})_\beta\langle f_x\rangle^\beta + \varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\langle g_x\rangle^\sigma = 0, \tag{A8}$$

we get

$$\varepsilon_\beta(\rho c_\mathrm{p})_\beta A - \varepsilon_\sigma(\rho c_\mathrm{p})_\sigma B = \varepsilon_\beta(\rho c_\mathrm{p})_\beta\left(\frac{\gamma\beta}{24}-\frac{9}{160}\right)+\varepsilon_\sigma(\rho c_\mathrm{p})_\sigma\frac{\gamma_\beta}{24}\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2. \tag{A9}$$

The value of A can be obtained by solving the system of equations (A5) and (A9)

$$A = -\frac{5}{32}+\frac{9}{40}\gamma_\beta-\frac{\gamma_\beta^2}{12}-\frac{\gamma_\beta(1-\gamma_\beta)}{12}\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2. \tag{A10}$$

We can now find the resulting macroscopic transport coefficient K_{xx}

$$K_{xx} = (\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma) - \varepsilon_\beta(\rho c_\mathrm{p})_\beta\langle uf_x\rangle^\beta. \tag{A11}$$

We begin by determining $\langle uf_x\rangle^\beta$ and the result is simply

$$\langle uf_x\rangle^\beta = \varepsilon_\beta^2 Pe\langle u\rangle^\beta H\left(\frac{39}{1120}-\frac{\gamma_\beta}{40}+A\right). \tag{A12}$$

Thus, after substitution we finally obtain

$$K_{xx} = k_\parallel + \varepsilon_\beta^3 Pe^2 k_\beta\left[\frac{17}{140}-\frac{\gamma_\beta}{5}+\frac{\gamma_\beta^2}{12} + \frac{\gamma_\beta(1-\gamma_\beta)}{12}\frac{\alpha_\beta}{\alpha_\sigma}\left(\frac{\varepsilon_\sigma}{\varepsilon_\beta}\right)^2\right] \tag{A13}$$

where $k_\parallel = (\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma)$.

Appendix B

Solving the system of equations for temperatures T_β and T_σ for a Dirac impulse of heat both in time and space at the interface β–σ of two semi-infinity media

$$\frac{\partial T_\beta}{\partial t} = \alpha_\beta\frac{\partial^2 T_\beta}{\partial y^2}$$

$$\frac{\partial T_\sigma}{\partial t} = \alpha_\sigma\frac{\partial^2 T_\sigma}{\partial y^2} \tag{B1}$$

along with the boundary conditions

$$T_\beta = T_\sigma \quad \text{at } y = 0 \tag{B2}$$

$$T_\beta = 0 \quad \text{at } y \to -\infty \tag{B3}$$

$$T_\sigma = 0 \quad \text{at } y \to -\infty \tag{B4}$$

$$k_\beta\frac{\partial T_\beta}{\partial y} = k_\sigma\frac{\partial T_\sigma}{\partial y}Q\delta_{t=0} \quad \text{at } y = 0 \tag{B5}$$

we get the total energy distribution

$$\frac{Q_\beta}{Q} = \int_{-\infty}^{0}\frac{(\rho c_\mathrm{p})_\beta}{\sqrt{\pi t}\left(\sqrt{(\rho c_\mathrm{p})_\beta k_\beta}+\sqrt{(\rho c_\mathrm{p})_\sigma k_\sigma}\right)} \times \exp\left(-\frac{y^2}{4\alpha_\beta t}\right)\mathrm{d}y = \frac{\sqrt{(\rho c_\mathrm{p})_\beta k_\beta}}{\sqrt{(\rho c_\mathrm{p})_\beta k_\beta}+\sqrt{(\rho c_\mathrm{p})_\sigma k_\sigma}} \tag{B6}$$

and

$$\frac{Q_\sigma}{Q} = \int_{0}^{+\infty}\frac{(\rho c_\mathrm{p})_\sigma}{\sqrt{\pi t}\left(\sqrt{(\rho c_\mathrm{p})_\beta k_\beta}+\sqrt{(\rho c_\mathrm{p})_\sigma k_\sigma}\right)} \times \exp\left(-\frac{y^2}{4\alpha_\sigma t}\right)\mathrm{d}y = \frac{\sqrt{(\rho c_\mathrm{p})_\sigma k_\sigma}}{\sqrt{(\rho c_\mathrm{p})_\beta k_\beta}+\sqrt{(\rho c_\mathrm{p})_\sigma k_\sigma}} \tag{B7}$$

This time-independent distribution gives the probability for a given particle located at the interface to jump either into the β-phase or into the σ-phase.

The same result may be obtained by solving a two-dimensional problem with a point source at the β–σ interface.

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