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Calculation of the interfacial heat transfer coefficient in porous media employing numerical simulations

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ABSTRACT

Numerical experiments in multiple representative elementary volumes (REVs) were conducted to validate calculations of macroscopic parameters for porous media models carried out employing a unit periodic cell (single REV). The simulation of a microscopic flow that develops through a porous medium formed by staggered square cylinders is presented to that purpose. A laminar steady flow regime is considered together with Péclet numbers in the $1–10^3$ range and porosities between 55 and 95%. In particular, the interfacial heat transfer coefficient (h_{sf}) is analyzed by comparing results found in literature with those reported here. First, the outlet boundary condition that is generally employed in single REV simulations for the case of constant wall temperature was tested by comparing the values it imposes in the flow with those obtained far away from the outlet (unperturbed). It was found that this outlet boundary condition is adequate and moreover, that the flow rapidly develops to satisfy it (one or two REVs in simulated cases). Additionally, two definitions found in the literature to calculate the h_{sf} were compared, and it was shown that both calculations differ in approximately 20% for the 55% porosity case and still present significant differences (>5%) for greater porosities. The h_{sf} coefficient was also calculated as a function of the REV's positions in the porous structure to show that it is position dependent or, in other words, it shows pore scale fluctuations. Therefore, it is concluded that single REV simulations are, in general, not sufficient to compute the parameter. A double average that filters pore scale fluctuations was employed and differences between this quantity and those obtained in a single REV were quantified. The results show these differences are small (<2%) for $Pe > 100$ but differences can be up to 15% for $Pe = 10$ or larger, for lower Pe numbers. Finally, a method that allows capturing the pore scale fluctuation of the parameter by employing single REV values was proposed. This method can be employed to calculate the double average of the h_{sf} coefficient for other boundary conditions, or to calculate other macroscopic parameters, such as the thermal dispersion coefficients.

1. Introduction

The analysis of heat transfer in porous media has attracted the research community for decades, possibly, due to the vast number of fields where it is needed (i.e. chemical, nuclear and mechanical to mention some examples). Applications of these fields, such as heat exchangers or metal foams, are systems characterized by large areas employed to transfer heat efficiently. These rather complex systems from the geometrical point of view (i.e. large number of tubes or pores) are generally modeled as homogeneous media to simplify a problem that involves multiscale physics. Thus, the heat transfer is not explicitly modeled at the pore scale, and the main interest is to calculate the amount of heat transfer at an intermediate scale between the scale of the system and that of the pore.

Homogeneous or porous media models have the great advantage to avoid the explicit representation of the pore scale, but they require unknown parameters to realistically model the physics that they do not explicitly represent. For instance, one of the relevant parameters regarding the heat transfer phenomenon, is the interfacial heat transfer coefficient (h_{sf}, [1] page 397) which accounts, in a macroscopic or average sense, for the heat transferred between different faces (e.g. solid and fluid) or parts of a system (e.g. primary and secondary circuits). During the last four decades, much effort was devoted to measure this parameter experimentally for different flow conditions, different fluids and different geometries in porous media [2]. Nowadays, extensive research is also focused in numerically computing the h_{sf} coefficient for different flow conditions, geometries, and fluid parameters, and more

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Nomenclature

h_{sf}	interfacial heat transfer coefficient
k_f	fluid thermal conductivity
p	pore length scale
D	square-edge length
H	REV's dimension (REV volume = $2H \times H$)
H_f	fluid cross section
Pe	Péclet number
Pe_D	Péclet number based on the Darcy velocity and D
Re	Reynolds number
Re_D	Reynolds number based on the Darcy velocity and D
q	wall heat flux
T_B	bulk temperature
T_w	wall temperature
U_D	V-normalized space averaged streamwise velocity, Darcy velocity
U	cross-section averaged streamwise velocity
V	volume of the REV
V_f	fluid volume inside the REV

Greek symbols

ε	local coordinate
ϕ	porosity
v	kinematic fluid viscosity

Additional notations

$\langle\rangle^{sf}$	intrinsic average
$\overline{\overline{\langle\rangle}}$	double average

importantly, in analyzing the adequate use of this coefficient in the macroscopic models described by partial differential equations.

Numerical simulations have gained popularity as a reliable tool to calculate macroscopic parameters. They are often carried out in periodic and simple porous structures that allow extracting a rich variety of results (e.g. laminar and turbulent flows and large range of porosities) with an acceptable computational cost [3,4]. The h_{sf} coefficient has not been an exception; for instance, Martin et al. [5], numerically determined this coefficient (or, more precisely, the Nusselt number) considering a porous structure represented by a periodic and triangular array of cylinders, and Kuwahara et al. [6] carried out numerical simulations in periodic arrays of staggered square rods for a large range of flow conditions ($1 < Re_D < 10^4$), porosities ($0.36 < \phi < 0.91$) and a variety of Prandtl numbers. To compute the h_{sf} coefficient based on numerical results in a periodic representative elementary volume (REV), both studies [5,6] employed a method where the interface solid–fluid was keep at a constant temperature. However, Kuwahara et al. [6] explicitly proposed an outlet boundary condition (BC) for the temperature field making an analogy between the periodic REV and the classical problem of force convection in a channel flow with constant wall temperature. After this study [6], different researchers advanced in the computation of the h_{sf} coefficient for different geometries, flow conditions and fluid parameters, together with different BCs at the interface or even with a volumetric heat source in the solid face [7–9]. Nevertheless, all these studies were based on simulations of a single periodic REV, and even, some studies such as that of Saito and de Lemos [7] employed alternative definitions to compute the h_{sf} coefficient. The present work, will discuss if the simulation of a single periodic REV is sufficient to obtain realistic macroscopic parameters, and will analyze the impact of the alternative definitions employed to compute the h_{sf} coefficient.

The main objective of this study is to gain insight in the validity of the procedure generally employed to obtain the h_{sf} coefficient from the simulation of a single periodic REV for a constant wall temperature. Still, the conclusions drawn from this work can be applied to different flow conditions or even in the calculation of other macroscopic parameters (e.g. dispersion coefficients). The first issue to be discussed is the validity of the outlet BC generally employed for the temperature field in single REV simulations. This condition has been suggested by Kuwahara et al. [6] and is a natural extension from the channel flow case. However, it is necessary to test if it is not artificially imposed in the flow. The second aspect to be discussed is the influence of the different definitions found in the literature in the quantification of the macroscopic parameter h_{sf}. Studies have either used intrinsic volume average values, or logarithmic means of bulk temperatures to compute the value of h_{sf}. Therefore, it is of interest to quantify the difference between both definitions, if any, and to analyze them from the physical point of view. The last aspect to be discussed, and possibly the most relevant one, is the influence of the REV location in the porous structure in the calculation of the macroscopic parameter. In this study, it will be shown that this aspect influences the result and therefore, special considerations have to be taken into account when a single REV simulation is employed.

The proposed tasks are achieved analyzing numerical results of the simulation of a clear flow stream that enters to a porous medium formed by staggered square rods. After a short distance (a few REVs) the flows develops and achieves a fully developed state that allows the comparison with single REV simulations. The present work first describes the computational domain and the numerical method employed. It follows the discussion related to the validity of the outlet BC that is generally employed for temperature. Next, numerical results are processed using different formulas found in the literature to calculate h_{sf} and differences are presented as a function of the geometry and flow conditions. Finally, the dependence of the macroscopic parameter on the REV location in the porous structure is evaluated and a new method to compute the macroscopic parameter based on single REV results is proposed.

2. Numerical method and domain of study

A schematic diagram of the domain selected for the simulation is shown in Fig. 1. The fluid flows from left to right, entering the porous medium after flowing a distance of $2H$ as a clear flow. The porous medium extends for a distance equal or greater than $16H$ depending on the flow conditions, making the length of the domain in the streamwise direction larger than $18H$ (i.e. eight REVs in a row). To save computational time, only the bottom half of the REV ($H/2$) was simulated. This simplification is based on the fact that simulations of a single REV with periodic BCs evolve to steady solutions at the Re numbers simulated in this study [10,11].

The governing equations for the fluid phase (mass, momentum and energy respectively) are given as follows:

$$\nabla \bullet \vec{u} = 0, \tag{1}$$

$$\frac{\partial \vec{u}}{\partial t} + (\nabla \vec{u}) \bullet \vec{u} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \vec{u}, \tag{2}$$

$$\frac{\partial T}{\partial t} + \nabla \bullet (\vec{u} T) = \frac{1}{Pe} \nabla^2 T. \tag{3}$$

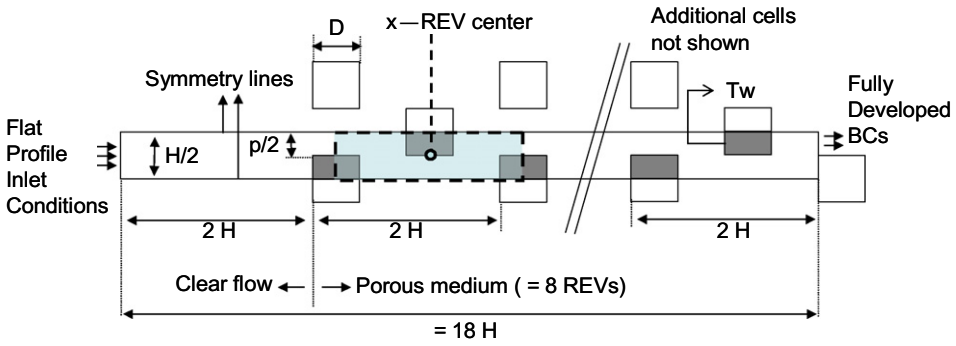

Fig. 1. Geometry of the domain simulated for the case of a free stream entering the porous medium ($18H \times H/2$).

Boundary conditions are standard for all the boundaries of the domain, except at the outlet, where periodic BCs are applied. On the solid walls BCs resume:

$$\vec{u} = \vec{0}, \quad T = T_w. \tag{4}$$

On the inlet of the domain (uniform field):

$$\vec{u} = (p/H, 0), \quad T = T_i. \tag{5}$$

On the bottom and top horizontal lines of the domain (symmetry):

$$\nabla_n \vec{u} = \vec{0}, \quad \nabla_n T = 0. \tag{6}$$

And on the outlet of the domain (periodicity):

$$\vec{u}(x_o, y) = \vec{u}(x_o - 2H, y), \tag{7}$$

$$T(x_o, y) = T_w + \tau(T(x_o - 2H, y) - T_w), \tag{8}$$

where x_o indicates to the x-coordinate of the outlet; and τ is defined as:

$$\tau = \frac{T_B(x) - T_w}{T_B(x - 2H) - T_w}, \tag{9}$$

where T_B is the bulk temperature of the fluid.

Eq. (8), the periodicity for temperature, may not be familiar for the reader and will be discussed in more detail in the following section.

To solve the set of Eqs. (1)–(3) under BCs given in Eqs. (4)–(8) the SIMPLER algorithm developed by Patankar [12] was employed. To model the diffusion and the convective terms, the central difference and the QUICK scheme were employed, respectively [13,14]. To evolve the initial condition to the steady state a backward Euler scheme was used. The solver has been fully tested and validated for different geometries, including those presented in this study [10,11]. Periodic variables were solved in an iterative manner, and profiles at the outlet were obtained from previous time steps according to Eqs. (7) and (8). Simulations were considered to reach convergence when normalized residuals were lower than 10^{-6}. It has been carefully checked that numerical solutions conserve energy in a global sense (domain) and in local sense (REV); additional details are available in [10].

The domain was discretized using a uniform and structured grid of squares, and a systematic grid refinement study was carried out. Macroscopic quantities reported in this study were found to be independent of any further grid refinement [10]. The grid resolution employed for each REV was 180×45 ($2H \times H/2$, streamwise x vertical direction), 128×32 and 180×45 for 55, 75 and 95% porosity respectively.

The Re number (based on the flow rate Up/ν) was varied between 1 and 335 depending on the porosity. The Pe number (defined as $Re \cdot Pr$) was varied from 1 to 1000. Three different porosities were simulated 55, 75 and 95%. It is important to note that to compare results with available data the Re number based on the Darcy velocity and size of the obstacles Re_D ($Re_D = Re\sqrt{1-\phi}$) is also used.

3. Results and discussion

3.1. Evaluation of the periodic boundary condition for temperature

The outlet BC for temperature (Eq. (8)) has been usually employed in single REV periodic simulations [7,9] as originally proposed in [6]. This last study showed that single REV simulations with a constant wall temperature are analogous, with regards to the outlet BC, to the case of force convection in a channel with a constant wall temperature. Eq. (8) is based on the well known fact that in a channel with a constant wall temperature, fully developed conditions are established [15] and that corresponds to:

$$\frac{\partial}{\partial x}\left[\frac{T(x,y) - T_w}{T_B(x) - T_w}\right] = 0. \tag{10}$$

This condition has been appropriately adapted for a REV like the one used in this study (Fig. 1). That is, one may expect that the temperature profiles are similar in the fully developed region by taking into account the periodicity of the geometry. Equation (10) takes meaning for the domain shown in Fig. 1, if x is taken in discrete points separated by a $2H$ distance (or more general, separated by the periodicity of the geometry). Therefore, Eq. (10) can be rewritten following these ideas as:

$$\frac{T(x - 2H, y) - T_w}{T_B(x - 2H) - T_w} = \frac{T(x,y) - T_w}{T_B(x) - T_w}, \tag{11}$$

which is an equivalent to Eqs. (8), (9). Although Eq. (11) has been used frequently, to the knowledge of the authors there is no proof that it is valid for a domain like the one considered in this study. The objective of this section is to test the validity of Eq. (11) with the use of numerical results.

Consider the domain shown in Fig. 1. The fluid enters to the porous medium and the flow and temperature fields develop rapidly to values unaffected by the outlet BC. The outlet is far away in the sense that the flow is more affected by the local obstacles and upstream conditions than by the outlet BC. Therefore, it is possible to compute both sides of Eq. (11) to evaluate the validity of that equality. With this purpose, a quantity F, which measures the accuracy of such equality, is defined:

$$F(x) = \frac{2}{H_f(x)} \int_0^{H_f(x)/2} \left| \frac{T(x,y) - T_w}{T_B(x) - T_w} - \frac{T(x + 2H, y) - T_w}{T_B(x + 2H) - T_w} \right| dy, \tag{12}$$

where H_f indicates the fluid spanwise section of the domain.

The quantity F, together with τ (Eq. (9)), are computed for different flow conditions ($10 < Pe < 1000, Re = 100$) and for different geometries ($0.55 < \phi < 95$). Fig. 2(a) shows computed values for F.

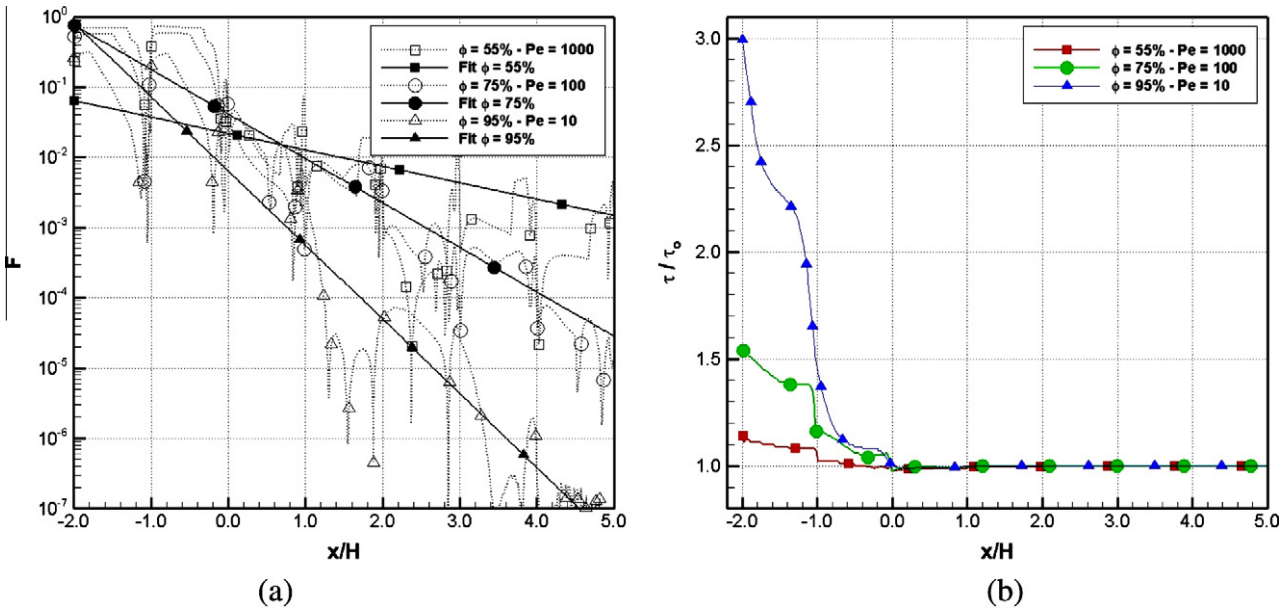

Fig. 2. F and τ as a function of the horizontal coordinate. (a) F, with porosity and Pe as parameters ($Re = 100$). (b) τ, with porosity and Pe as parameters ($Re = 100$). Note that τ_o is the value at the outlet.

It is found that F goes rapidly to zero (after a few REVs) showing that the fully developed condition is rapidly established and that, Eq. (11) or the BC given in Eq (8), is effectively adequate for the case under study. Note that because F is strongly dependant on the horizontal coordinates, an exponential fit has been added to clearly show the trend of the values. Note also that x/H in Fig. 2 corresponds to the horizontal coordinates shown in Fig. 1; that is, $x/H = -2$ is the inlet boundary.

Additionally, it is important to point out that τ is constant, independent of x, showing, as expected, an exponential decay of the quantity $T_B(x) - T_w$ if x is taken again in discrete points separated by a $2H$ distance. This claim is supported by Fig. 2(b) that shows that τ/τ_o goes rapidly to one (τ_o is the value at the outlet). Therefore, the BC can be rewritten to express the temperature in the fully developed region as:

$$T(x,y) = T_w + \tau(T(x-2H,y) - T_w), \tag{13}$$

where τ is constant. This result shows that, in the fully developed region, the value of the temperature in a single REV is enough to know the value of the temperature in this entire region. This finding will be used in the following sections.

3.2. Calculation of h_{sf} from different definitions

As it was mentioned in the introduction, the h_{sf} coefficient is of great importance to complete the macroscopic porous media model as it accounts for the heat transferred between the solid and fluid faces at macroscopic scales. Its definition is generally given as [1]:

$$h_{sf} = \frac{\frac{1}{V}\int_{A_{sf}} k_f \nabla T \cdot d\vec{A}}{a_i\left(\langle T_w\rangle^s - \langle T\rangle^f\right)}, \tag{14}$$

where V is the REV volume, A_{sf} is the interfacial area inside the REV and a_i is the interfacial area per unit volume A_{sf}/V. Note that with the numerical results obtained in domains as the one shown in Fig. 1, the value of h_{sf} can be computed evaluating Eq. (14) in a REV of $2H \times H/2$.

Eq. (14) shows two important features. First, the numerator represents all the energy interchanged between the fluid and the solid inside the REV (term that appears in macroscopic models, see for example [6]). And second, the modeling of this energy is given by the coefficient times the difference between dependant variables of the macroscopic model (i.e. macroscopic values of temperature or denominator of the r.h.s. of Eq. (14)). This allows to naturally incorporating the model in the macroscopic equations.

But, an alternative definition has been employed in the literature to compute de value of the h_{sf} coefficient (e.g. [7]) that makes use of the logarithmic mean temperature, defined as:

$$h_{sf} = \frac{\frac{1}{V}\int_{A_{sf}} k_f \nabla T \cdot d\vec{A}}{a_i \Delta T_{ml}}, \tag{15}$$

where the logarithmic mean is calculated as:

$$\Delta T_{ml} = \frac{T_B|_{inlet} - T_B|_{outlet}}{\ln\left[(T_w - T_B|_{outlet})/(T_w - T_B|_{inlet})\right]}, \tag{16}$$

and the subscripts inlet and outlet refer to the boundaries of the REV. This definition may have its origin in the useful result found for the force convection in a channel with a constant wall temperature. In this problem, the logarithmic mean temperature is the adequate mean to compute the heat transferred in a given length of the channel. Or, in other words, the logarithmic mean has to be employed to obtain a constant heat transfer coefficient in the fully developed region.

To model the heat transferred in the REV under consideration, it may be accepted that Eq. (15) is not ready to be employed in a macroscopic model because the logarithmic mean is not known (note that ΔT_{ml} is computed using T_B and the macroscopic model uses $\langle T\rangle^f$). Moreover, one may argue that from the macroscopic point of view, Eq. (14) defines a local value of h_{sf} and therefore, the local temperature difference (i.e. $\langle T_w\rangle^s - \langle T\rangle^f$) should be employed to compute a constant value of the coefficient. That is, Eq. (14) represents a point in the macroscopic sense, not only for h_{sf} but also for the heat transferred in the REV and for the intrinsic average of the temperature. Additionally, it can be considered that in the constant wall temperature channel, if the local heat flux is known, the value of the convective coefficient can be computed as this value over a temperature difference.

Despite the before mentioned discussion, in order to analyze if the different definitions of h_{sf} produce different estimations of the

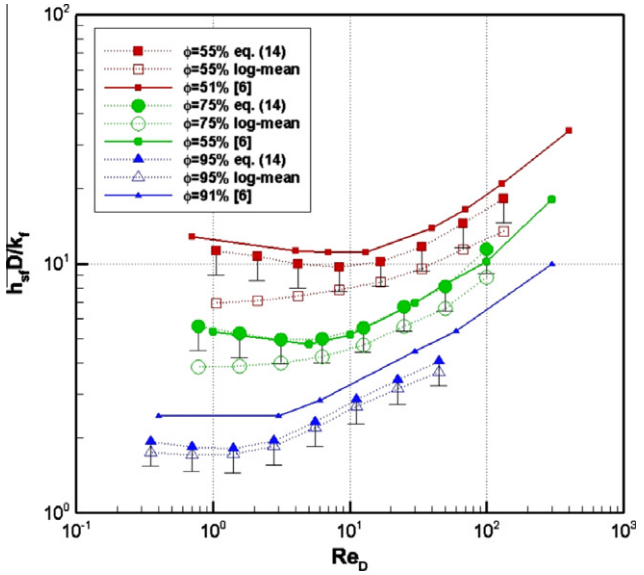

Fig. 3. h_{sf} calculated from Eqs. (14) and (15) (log-mean) for 55, 75% and 95% porosity. A 20% error bar is plotted from the data computed with Eq. (14). Data from reference [6] is added for comparison purposes.

parameter, the difference between the values obtained from Eqs. (14) and (15) were quantified by computing them with the results obtained by employing a fixed REV like the one shown in Fig. 1 in the fully developed region. Fig. 3 shows the coefficient calculated with Eqs. (14) and (15), as a function of Re_D and with the porosity as a parameter. The Pr number is constant and equal to 1 making $Pe_D = Re_D$. The results obtained by Kuwahara et al. [6] are included for validation purposes. It is important to note that the numerator in Eq. (14) is computed based on the conduction heat flux integrated over the walls of the REV. An energy balance based only on the inlet–outlet bulk temperature in the REV is not adequate for low Pe numbers as it neglects, or assumes of equal magnitude, conduction through the inlet and outlet boundaries of the domain.

The results presented in Fig. 3 show that the definition given in Eq. (15) is always lower than that given in Eq. (14). Differences greater than 20% are found at low porosities and low Re_D numbers. A 20% error bar is included to easily obtain an idea of the difference between both values in the log scale. In conclusion, it is recommended to employ the definition given in Eq. (14) to calculate the parameter of interest. This is not only because it is the theoretically adequate value to use in macroscopic models but also, because if Eq. (15) is used it may differ significantly from the correct definition.

The comparison with the data extracted from reference [6] is excellent at 75% porosity and shows the right trend at the other two porosities. However, it is important to mention that results from [6] have been normalized according to the suggestion given in [16]. Gamrat et al. [9] carried out numerical simulations to calculate the interfacial coefficient in a geometry, and with conditions similar to those employed by [6]. Results between both studies were different. Further, [16] carried out a third independent calculation to show that Kuwahara's results and the other two independent calculations differ in a factor of two. Therefore, in this work, Kuwahara's results have been multiplied by two for comparison.

3.3. Calculation of h_{sf} using different REV positions

A genuine question in the calculation of macroscopic parameters, such as the h_{sf}, may be considered when a single REV with periodic BCs is employed: is the parameter independent of the position chosen to locate the REV in the porous structure? For instance, for the artificial porous medium employed in [6], the REV is taken as the one indicated in the left panel of Fig. 4 (i.e. symmetric respect to the center of the REV). Other studies, however, have employed the REV shown in the right panel to calculate macroscopic parameters [17]. The purpose of this section is to discuss the influence of the REV position in the calculations of macroscopic parameters.

The numerical simulations presented here allow to gain insight on the subject under consideration because h_{sf} can be computed as a function of the horizontal coordinate. Fig. 5 shows the value of h_{sf} for different fluid properties (Fig. 5(a)) and for different porosities (Fig. 5(b)), as a function of the REV position (note that the abscissa corresponds to the center of the REV as indicated at the top of the Figure). The results show a periodic signal with period H with a notorious peak that is larger in the low porosity range and in the low Pe number range. This peak can be easily explained considering that when the REV is moving, for example, to the right, there are regions in which the interface solid–fluid is fixed. Thus, the numerator in Eq. (14) is constant while the temperature difference $\langle T_w\rangle^s - \langle T\rangle^f$ decreases exponentially by conduction and convection of energy through the fluid vertical boundaries of the REV.

The results shown in Fig. 5 indicate that special care is needed when macroscopic parameters are computed based on single REV simulations. For the cases simulated here, different REV selections may yield results that differ up to 100%. Therefore, a procedure to compute values independent of the REV positions is needed; or at least, a procedure to quantify the error that can be incurred if single REV simulations are employed. The answer to this aspect is found in the concept of cellular average defined and discussed in great detail by Quintard and Whitaker [18,19]. In general words, they discuss the importance of considering an average depending on the particular porous medium and showed with a simple example, that the intrinsic average is generally not adequate for periodic media as it contains pore scale fluctuation as those found in Fig. 5. In particular, for periodic media as the one considered in this study, a double volume average is the correct average because it filters pore scale fluctuations (this is equivalent to employ a triangular shaped weighing function [19]). This double average over the REV can be understood as a second average over the signals shown in Fig. 5. Clearly, the averaging of this periodic signal over a $2H$ distance will result in a constant, independent of x, value. In other words, this second average filters REV scale oscillations

The double average is then recommended and will be computed and compared with the single REV results. As it was mentioned, it is of interest to quantify the difference between both averaging procedures. Table 1 shows the double average value and the percent difference that is obtained respect to that calculated with a single REV (employing the REV location shown in Fig. 4(a)). Three different porosities (55% in Table 1(a), 75% in Table 1(b) and 95% in Table 1(c)), and a large range of Re_D and Pe numbers are included in Table 1. Note that for the 55% porosity case, the $Pe = 1$ condition is not shown because the fluid temperature reaches the wall temperature in less than one REV distance, to the machine precision.

Table 1 shows differences no larger than 17% in all the cases under study. Greater differences are found for low porosities and low Pe numbers. The single REV shown in Fig. 4(a) has been chosen in the majority of the studies reviewed, and represents a good selection as it yields results close to the double average value for the calculation of h_{sf}. In particular, in the large Pe number range (>100), it can be considered an excellent approximation to the double average value.

4. Computation of double averaging employing single REV simulations

In Section 3.3 it was shown that single REV simulations yield results that are REV position dependant. Based on Fig. 5, it can be said

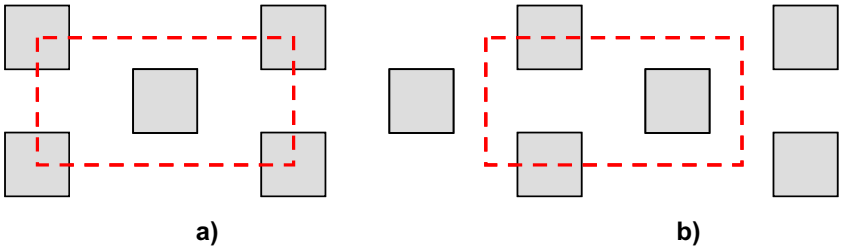

Fig. 4. Two possible REV locations in the porous structure. (a) Employed in [6]. (b) Employed in [17] to compute thermal dispersion coefficients.

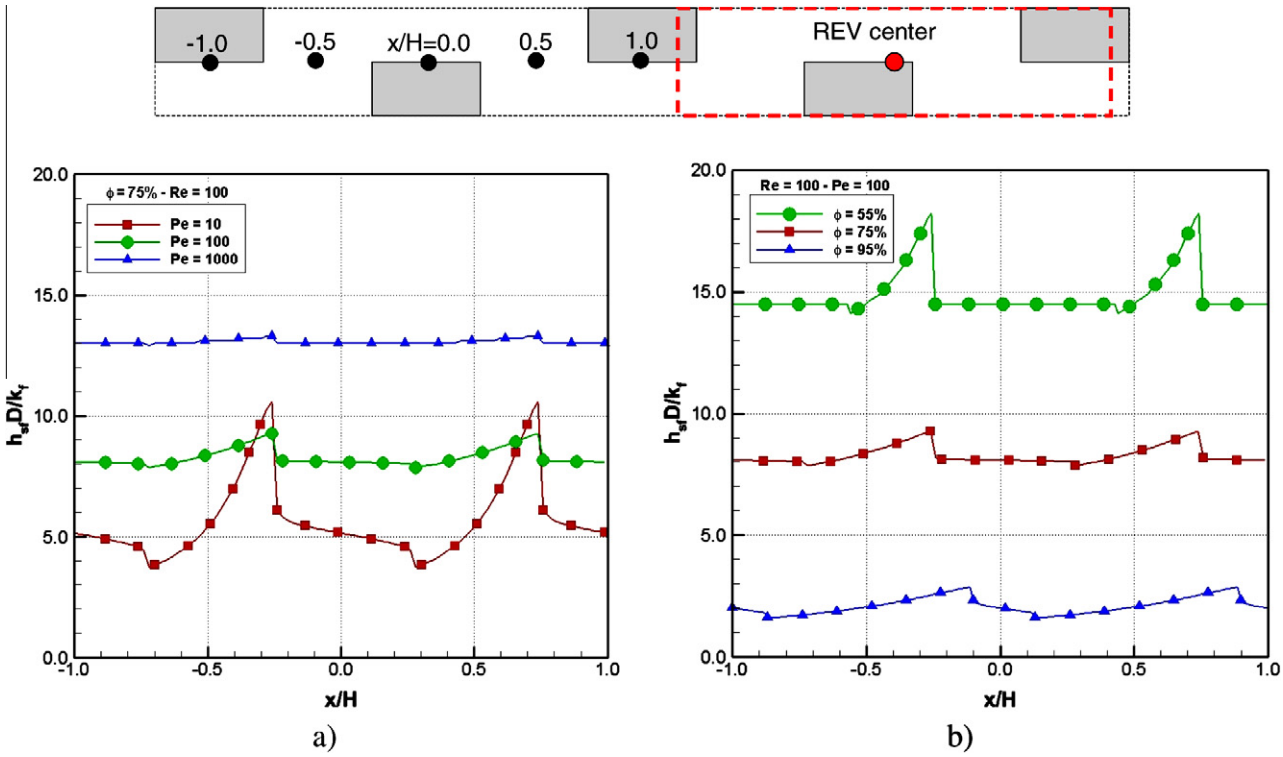

Fig. 5. h_{sf} as a function of the REV position. (a) For different *Pe* numbers. (b) For different porosities. Note that the abscissa, x/H, corresponds to the center of the REV.

Table 1
Double average values for h_{sf} and percent difference respect to a single REV calculation. (a) 55% porosity. (b) 75% porosity. (c) 95% porosity.

(a)	*Pe*					
	10		100		1000	
Re_D	h_{sf}	1-REV% diff.	h_{sf}	1-REV% diff.	h_{sf}	1-REV% diff.
1	10.59	−8.3	12.37	−1.6	16.91	−0.2
10	10.77	−9.5	12.68	−1.9	17.28	−0.3
75	11.66	−13.9	14.98	−2.6	23.00	−0.4

(b)	*Pe*							
	1		10		100		1000	
Re_D	h_{sf}	1-REV% diff.	h_{sf}	1-REV% diff.	h_{sf}	1-REV% diff.	h_{sf}	1-REV% diff.
1	6.65	−13.1	5.16	−5.1	6.79	−1.2	9.50	−0.2
10	6.93	−16.5	5.32	−6.8	7.17	−1.7	10.04	−0.3
75	6.86	−16.6	5.72	−9.7	8.38	−2.3	14.50	−0.4
(c)								
1	1.99	−0.5	1.91	−2.6	2.82	−1.0	4.30	−0.2
10	2.03	−1.6	2.04	−4.3	3.20	−1.6	4.79	−0.3
75	2.02	−0.6	2.12	−4.8	3.56	−2.0	5.81	−0.3

that simulations that consider at least one and a half REVs in the streamwise direction should be employed to obtain the pore scale variation of the macroscopic parameter and therefore, to compute the double average value. This result is discouraging in the sense that a numerical solution more expensive than that for a single REV is needed. However, this costly simulation can be avoided by

the fact that the temperature in the fully developed region is periodic in the sense of Eq. (13). With a single REV simulation, the parameter τ can be computed. Thus, the temperature is already known in the entire fully developed region based on the known values. If x belongs to the resolved single REV region, the temperature is:

$$T(x+n2H,y) = T_w + \tau^n (T(x,y) - T_w), \tag{17}$$

where n is an integer ($\geqslant 0$). Additionally, and noting that the heat flux in the REV-walls is proportional to the temperature gradient normal to the wall, the heat flux can be readily known for the entire fully developed region based again, on the values known from the single REV simulation. Therefore, the temperature gradient normal to the wall can be calculated employing Eq. (17) to yields:

$$q''(x+n2H,y)|_{wall} = \tau^n q''(x,y)|_{wall}, \tag{18}$$

where $q''(x,y)|_{wall}$ is the heat flux at any point of the solid–fluid interface of the REV simulated and n is an integer ($\geqslant 0$).

Eqs. (17) and (18) allow computing the pore values for the temperature and heat flux in the entire fully developed region based on 1-REV results. Therefore, taking into account the particular geometry of the porous medium, the pore scale dependency of the macroscopic parameter can be computed as:

$$h_{sf}(x) = \frac{\frac{1}{V}\int_{A_{sf}(x)} q''(x+\varepsilon,y)\cdot d\vec{A}_\varepsilon}{a_i(\langle T_w\rangle^s - \frac{1}{V_f(x)}\int_{V_f(x)} T(x+\varepsilon,y)dV_\varepsilon)} = \frac{1}{a_i}\frac{\langle Q\rangle(x)}{[\langle T_w\rangle^s - \langle T\rangle^f(x)]}, \tag{19}$$

where the local coordinate ε belongs to the REV and $\langle Q\rangle$ is the volume average heat flux. Equation (19) can be easily averaged in the REV to obtain a constant double average value as:

$$\overline{\overline{h_{sf}}} = \frac{\frac{1}{2H}\int_{2H}\langle Q\rangle(x)dx}{\frac{a_i}{2H}\int_{2H}[\langle T_w\rangle^s - \langle T\rangle^f(x)]dx}. \tag{20}$$

This simple method can be employed, for instance, to compute the double average of parameters such as the thermal dispersion coefficient. Moreover, it can be employed for different BCs than those used here, such as the case of constant heat flux.

5. Concluding remarks

Based on multiple REV numerical simulations, several aspects involved in the calculation of the macroscopic interfacial heat transfer coefficient were analyzed. First, the BC generally employed in single REV simulations was tested by comparing the values it imposes on the flow with those obtained in the fully developed region and unperturbed by the outlet. This test was performed for three different porosities (55, 75 and 95%) and for *Pe* numbers on the 10–10^3 range. It was found that the imposed BC is adequate and moreover, that the flow rapidly develops to satisfy it (one or two REVs in the simulated cases).

Additionally, it was recognized that the literature proposes two definitions to calculate the h_{sf} parameter. The one that employs the logarithmic-mean to carry out the calculation was not recommended as it is not ready to be used in macroscopic models and because it does not present any advantage on physical grounds. Moreover, it was shown that the calculation of h_{sf} using the two different definitions differ in approximately 20% for the 55% porosity case and still present significant differences (>5%) at greater porosities.

Finally, it was shown that the h_{sf} coefficient depends on the single REV location in the porous structure. In other words, h_{sf} shows fluctuations at the pore scale if it is computed based on volume averaged quantities. Therefore, it is recommended to employ double average values and, in cases where a single REV simulation has to be employed, special care should be taken to select the REV location in the porous structure. Differences between a double average and a single REV average (position shown in Fig. 4(a)) were quantified to show that they are small (<2%) for $Pe > 100$, they can reach 15% for $Pe = 10$ and they can be even larger for lower *Pe* numbers. To avoid the computation of more than a single REV, a method that allows capturing the pore scale fluctuation and employs single REV values was proposed. This method can be easily applied to calculate the h_{sf} coefficient for other BCs, or to calculate other macroscopic parameters, such as thermal dispersion coefficients.

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