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New framework for upscaling gas-solid heat transfer in dense packing

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Abstract:

The objective of this work is to provide a suitable upscaling framework for modeling gassolid heat transfer in dense packings. In a macroscopic two-temperature model, the pore-scale heat transfer is modeled by determining a Nusselt number. We introduce a new surface statistical filter to extract the Nusselt number from pore-scale simulations. A thermal offset boundary condition is developed to deal with dense packings that exhibit high heat transfer. The new method is applied to sphere packings. Several pore-scale simulations over a range of Reynolds number (10-100) and solid volume fraction (0.1-0.6) are performed. The extracted Nusselt numbers show very good agreement with results available in the literature for lower solid volume fractions (0.1-0.5). We show that the Nusselt number to be used with the twotemperature model is the Nusselt number correlation for a dense packing of spheres. Nevertheless, the propose a valid Nusselt number correlation for a dense packing of spheres. Nevertheless, the proposed scaling framework is not restricted to sphere packings.

Graphical Abstract:



Dependency of the Nusselt number based on mixing-cup temperature on the Reynolds number. The symbols are the pore-scale simulations results and the error bars indicate 95% confidence intervals. The lines are obtained from the Gunn correlation.

Keywords: Dense packed-bed, Nusselt correlations, upscaling, fixed-bed, heat transfer

Highlights:

- Homogenization framework for heat transfer calculations in porous media
- Robust temperature offset boundary condition for upscaling
- Pore-scale simulation to calculate heat transfer for a dense fixed bed
- Heat transfer link between microscale and macroscale for sphere packings

Nomenclature

Ren	particle Reynolds number
Pr	Prandtl number
Ri	Biot number
Nu.	filtered temperature Nusselt number
Num	mixing-cup temperature Nusselt number
Pe	Peclet number
$Nu(x,\omega)$	local filtered temperature Nusselt number
$Nu_m(x,\omega)$	local mixing-cup temperature Nusselt number
h	convective coefficient
x	streamwise location
L	computational domain length
D	particle diameter
a_f	thermal fluid diffusivity
a_s	thermal solid diffusivity
$ ho_f$	fluid density
$ ho_s$	solid density
C_{p_f}	fluid specific heat
C_{p_s}	solid specific heat
k_f	fluid conductivity
k _s	solid conductivity
\mathcal{E}_{f}	fluid volume fraction
\mathcal{E}_{S}	solid volume fraction
v_f	kinematic fluid viscosity
V	entire volume
V_f	fluid volume
A	entire spanwise surface
A_f	fluid spanwise surface
T_m	mixing-cup temperature
$T_{m,i}$	inlet mixing-cup temperature
$T_{m,o}$	outlet mixing-cup temperature
u_x	streamwise superficial fluid velocity
$\langle \psi_f \rangle$	ψ_f superficial volume average
$\langle \psi_f \rangle$	ψ_f intrinsic volume average
$\frac{\psi_f}{dr}$	ψ_f subgrid fluctuations
ψ_f	ψ_f superficial statistical surface average
$\overline{\psi_f}$	ψ_f intrinsic statistical surface average
A_{sf}	solid-fluid surface interface
Γ_{sf}	solid-fluid spanwise linear interface
r_h	heat ratio
J _h	heat offset
u d A	fluid velocity vector
uA dl	normal linear element vector
N	total number of realizations
ω	a particle configuration realization
	1 6

1. Introduction

Several industrial processes involve gas-solid heat transfer in a packed bed. In addition to the classical applications in the chemical or energy industries, some emerging technological processes rely on packed beds. These developing applications are, for example, CO₂ capture [1], biofuel production [2] [3], thermal energy storage (TES) [4] [5], concentrated solar power plant [6] [7] or advanced adiabatic compressed air energy storage (AA-CAES) [8] [9]. Accurate heat transfer prediction plays a major role in the design and control of these systems. However, their design requires expensive experiments that are not suitable for optimization. This explains the rise of CFD simulations, which are an excellent alternative. Nevertheless, the challenge remains to scale-up the heat transfer properties from the pore-scale, called the microscale, to the scale of the packed-bed, called the macroscale. **Fig. 1** illustrates the hierarchy of scales in a porous material. The representative elementary volume (REV) with the support scale is introduce as a spatial cut-off filter. Thus, volume averaging over the REV describes the pore-scale as a subgrid scale. Beyond the spatial filter, individual solids are no longer resolved. An upscaling method is needed to model the effect of unresolved scales on resolved scales.



Fig. 1 Illustration of the hierarchy of scales in a porous material. (a) A packed-bed with macroscale length L_M . (b) A representative elementary volume (REV) with support scale Δ . (c) A vertical slice through the medium with microscale D.

Several upscaling methods have been developed over the years [10]. At the pore scale, the heat transfer can be described by two energy conservation equations, one for the solid and one for the gas. The coupled equations involve a common boundary which is the solid-gas interface. On the one hand, a large-scale modeling effort has left out the detailed description of the interface. Instead, in this heuristic model, the interface is only described as an amount of surface. By analogy with classical solid-gas heat transfer, the heat flow is modeled by a temperature difference and a convective coefficient h. The dimensionless form of h is the Nusselt number Nu, which defines the ratio of convective to conductive heat transfer at a

boundary in a fluid. Therefore, upscaling method based on the heuristic model leads to the development of Nusselt number correlations [11] [12] [13] [14]. In contrast, the volume averaging method focuses on the effect of detailed interface geometry on heat transfer. The method is based on the volume averaging theory [15] [16] which introduces a spatial filter [17] for the momentum and energy equations. This method leads to a closure problem for a specific geometry of the porous medium. It has been derived for steady case by Quintard and Whitaker [18] and Koch and Brady [19]. Recently, it has been extended to unsteady case by Lasseux et al. [20]. A third approach consists in implicitly introducing the effect of the detailed geometry of the interface in the Nusselt number correlation. The mixed method applies the volume averaging method to the conservation equations and the closure terms are postulated using the classical heuristic method. These methods based on two energy conservation equations lead to two-temperature macroscopic models, namely the Schumann model or the continuous solid model [15]. Actually, almost every pore-scale simulations [21] [22] [23] [24] [25] [26] [27] [28] that attempt to extract Nusselt number from a piece of packed bed rely on the mixed method. However, since the upscaling framework is not properly defined, this leads to some indeterminacies in defining the appropriate boundary conditions, how to calculate the Nusselt number, or how the Nusselt number is consistent with the macroscopic two-temperature model [22]. As pointed out by Chen et al. [27], the adopted boundary conditions can have an impact on the numerically derived correlations. Moreover, as stated by Sun et al. [22], the Nusselt number is usually calculated for the mixing-cup temperature $T_m = \overline{u_x T_f} / \overline{u_x}$ but is used in the macroscopic two-temperature model with the average temperature \overline{T}_{f} . As a matter of fact, the widely used Gunn correlation [29] for calculating solid-gas heat transfer in a packed bed is based on the mixing-cup temperature.

In the literature, many Nusselt number correlations for sphere packings have been numerically derived for a range of solid volume fractions between 0.1 and 0.5 and a range of Reynolds numbers between 1 and 100, with Prandtl number of 0.7 or 1 [21] [22] [23] [24] [27]. However, very few studies manage to numerically derive correlations for dense packings [25]. Furthermore, aside from the work of Tenneti et al. [23] and Sun et al. [22], the boundary conditions used for the simulations are not consistent with the upscaling framework. As reported by Feng and Musong [30], the constant temperature imposed on the inlet leads to an entrance effect that produces a high transfer rate on the entrance particles. Although the thermally fully developed temperature condition proposed by Tenneti et al. [23] seems to be a good alternative, this condition suffers from numerical instability when the packing is dense and the particulate Reynolds number is low $Re_p = \overline{u_x}D/\nu_f$.

In the development of an AA-CAES system [31], accurate prediction of fixed bed heat transfer is necessary as it plays a key role in the design of the TES. This motivated us to provide a clarified framework to perform the heat transfer upscaling from the pore-scale to the packedbed scale. This paper is organized as follows. In Section 2, we describe the problem statement with the assumptions that have been made. In Section 3, we present the equations to be solved with the boundary conditions, in particular the thermal offset boundary condition introduced to deal with the dense packing simulations. In Section 4, we express the developed upscaling framework. We explain the filtering equation process, conditions, and methods for extracting the Nusselt number from the simulation. In Section 5, we present the results of the current methodology for $0.4 \le \varepsilon_f \le 0.8$ and $10 \le Re_p \le 100$ with Pr = 0.7. We compare our results and those of Gunn and Sun. Then, in section 6, we discuss the correct definition of the Nusselt number for the two-temperature model as well as the applicability limits of the current upscaling method. Finally, in section 7, we summarize our main results.

2. Problem statement

We define the problem statement and the simplification assumptions corresponding to the fixed beds encountered in practice. We summarize the simulation parameters and the method to obtain the particle assembly.

2.1. Pore-scale gas-solid heat transfer

We investigate the heat transfer between gas and solid for a monodisperse fixed assembly of spherical particles, as shown in Fig. 2. x is the streamwise direction and y, z are the spanwise directions. In the flow direction, a hot gas is introduced at the inlet x = 0. The gas is cooled by the cold particles. According to Wood et al. [32] for a Reynolds number below 100, we remain in the inertial regime. The Biot number $Bi = hD/k_s$ is the ratio between the convective heat flux of the fluid and the conductive heat flux of the solid. It indicates whether the thermal behavior of the solid is dominated by external convection or internal conduction. For a Biot number less than 0.1, the temperature gradient inside the solid is negligible. The temperature of the solid can be assumed to be constant throughout the volume of the material. In a practical packed bed, the size of the solid particles and the thermal conductivity generate a small Biot number Bi < 0.1. This allows us to assume a uniform temperature T_s of the particles. In addition, the time scale of the thermal response of the solid is about three orders of magnitude higher than the time scale of the fluid convection [23]. This allows us to assume that the temperature of the particles is constant. Furthermore, we neglect viscous dissipation, radiation and free convection as their contribution to heat transfer is very small outside the Stokes flow regime [23] for moderate temperature T < 600K. In addition, the fluid properties are assumed to be constant to allow simplification of the upscaling method. Given these assumptions, only the fluid phase needs to be simulated. The solid phase has a constant and uniform temperature $T_{\rm s}$ which is the boundary condition for the fluid phase.



2.2. Pore-scale geometry

To avoid the introduction of geometric anisotropy in the large-scale model, the geometry of the REV must be periodic. The REV is a periodic cube with a length L of five particles diameter (D). The discrete element method is used to generate the packing with the YADE software [33]. A tri-axial periodic compression for a given fluid volume fraction is

simulated. In addition, a stress-free stage is performed to produce non-overlapping packings. There are several possible particle packings for the same fluid volume fraction ε_f . Therefore, 8 packing realizations were generated for each fluid volume fraction. The simulated fluid volume fraction and Reynolds number are summarized in **Table 1**. The Prandtl number is 0.7.

\mathcal{E}_{f}	Rep
0.8	10, 20, 30, 40, 50, 80,100
0.6	20, 50, 100
0.4	20, 50, 100

Table 1 Simulated fluid volume fraction and Reynolds number

3. Numerical method

3.1. Equations

The inertial regime allows us to restrict the heat transfer problem to the steady state. Therefore, we solve the steady state Navier-Stokes equations for the fluid phase with constant fluid properties. The steady state energy conservation equation is added to the set of equations. Assuming no viscous dissipation, no radiation, and no free convection, the steady state fluid energy conservation equation is as follows:

$$\nabla \cdot (\boldsymbol{u}T_f) = a_f \nabla \cdot (\nabla T_f) \qquad \text{in } V_f$$

$$T_f = T_s \qquad \text{at } A_{sf}$$

$$u_f = 0 \qquad \text{at } A_{sf}$$
(1)

where $a_f = k_f/(\rho_f C_{p_f})$ is the thermal diffusivity. As mentioned in Section 2.1, only the energy equation for the fluid phase is solved with T_s as the boundary condition at the particle surface A_{sf} . At the REV boundaries, periodic boundary conditions are imposed for the fluid velocity. For temperature and pressure, periodic boundary conditions are imposed only in the spanwise directions. These conditions are summarized in equations (2).

$$u(0, y, z) = u(L, y, z)$$

$$u(x, 0, z) = u(x, L, z)$$

$$u(x, y, 0) = u(x, y, L)$$

$$T_{f}(x, 0, z) = T_{f}(x, L, z)$$

$$T_{f}(x, y, 0) = T_{f}(x, y, L)$$

$$P(x, 0, z) = P(x, L, z)$$

$$P(x, y, 0) = P(x, y, L)$$

(2)

It is shown in [34] that Navier-Stokes equation for incompressible flow with periodic boundary condition on the velocity leads to a constant jump condition on the pressure.

$$P(L, y, z) = P(0, y, z) - \lambda$$
(3)

However, the jump cannot be imposed because it is unknown. Instead, a fixed value P_0 is imposed at the inlet x = 0 and a zero gradient is imposed at the outlet x = L. These conditions are consistent with the condition in equation (3).

$$\frac{\partial P(L, y, z)}{\partial x}\Big|_{L} = \frac{\partial P_{0}}{\partial x}\Big|_{L} - \frac{\partial \lambda}{\partial x}\Big|_{L} = 0$$
(4)

In the streamwise direction, the gas is cooled by heat transfer with the particles. We present, in the section 3.2, a thermal offset boundary condition to account for the temperature decrease along the x axis.

3.2. Thermal offset boundary condition

We need to introduce a periodic thermal boundary condition with a temperature loss. Assuming a linear form for a modified periodic boundary condition, we can write:

$$T_f(0, y, z) - T_s = \alpha \left[T_f(L, y, z) - T_s \right] + \beta$$
(5)

where α and β are constants. Multiplying equation (5) by the axial fluid velocity, taking the spanwise surface integral,

$$\int_{y,z} u_x T_f(0, y, z) \, dy dz - \int_{y,z} u_x T_s \, dy dz = \int_{y,z} \left[\alpha \left[u_x T_f(L, y, z) - u_x T_s \right] + u_x \beta \right] dy dz \tag{6}$$

We define a surface filter as:

$$\bar{\psi} = \frac{1}{dydz} \int_{y,z} \psi \, dydz = \frac{1}{A} \int_{A} \psi \, dA \tag{7}$$

We divide the equation (6) by the flow rate velocity and use the surface filter notation:

$$\frac{\overline{u_x T_f(0, y, z)}}{\overline{u_x}} - T_s = \alpha \left[\frac{\overline{u_x T_f(L, y, z)}}{\overline{u_x}} - T_s \right] + \beta$$
(8)

We define the inlet mixing-cup temperature $T_{m,i}$ and the outlet mixing-cup temperature $T_{m,o}$ as:

$$T_{m,i} = \frac{\overline{u_x T_f(0, y, z)}}{\overline{u_x}}$$
$$T_{m,o} = \frac{\overline{u_x T_f(L, y, z)}}{\overline{u_x}}$$
(9)

The equation (8) writes:

$$T_{m,i} - T_s = \alpha [T_{m,o} - T_s] + \beta \tag{10}$$

At the inlet, the heat flux must be constant. The inlet mixing cup temperature should not depend on the outlet mixing cup temperature. There are two obvious solutions for the choice of constants α and β :

(1)
$$\begin{cases} \alpha = 1 \\ \beta = T_{m,i} - T_{m,o} = j_h \end{cases}$$
 (11)

(2)
$$\begin{cases} \alpha = \frac{T_{m,i} - T_s}{T_{m,o} - T_s} = r_h \\ \beta = 0 \end{cases}$$
 (12)

The solution (2) is the thermal condition expressed in [23], where $\alpha \equiv r_h$ is the heat ratio. This heat ratio is obviously an unknown quantity and is obtained by an iterative process. Similarly, solution (1) has an unknown heat offset $\beta \equiv j_h$ that must be obtained by an iterative process.

For high heat transfer in long boxes, the fluid temperature can be very close to equilibrium with the solid temperature at the end of the box. This leads to a high heat ratio, which in turn leads to a high value of the inlet temperature. This behavior increases the numerical instability for low Reynolds number and high-density packing cases. This may explain the discrepancy in the PR-DNS data in [35] on the exponential decay behavior of the mixing-cup temperature for low Reynolds number. Therefore, the solution (1) with the heat offset is preferred. The developed thermal boundary condition is numerically robust and based on a rigorous framework. This provides another explanation for the thermal boundary condition developed in [23], originally based on the similarity with pipe flow.

3.3. Workflow and finite volume solver

The geometry of the spheres was introduced into OpenFOAM's snappyHexMesh mesher through searchable sphere objects. We used the buoyantSimpleFOAM solver [36] of OpenFOAMv1712 to solve for momentum, mass and energy conservation of the fluid. We implemented the thermal boundary offset condition defined in Section 3.2 and the convergence controllers of the SIMPLE algorithm have been modify to account for the convergence of the heat offset j_h . We used a second order discretization scheme for convective terms with the *linearUpwind* [37] scheme. For the diffusive terms, we used the second order scheme *Gauss linear* [38]. According to [39], the momentum boundary-layer thickness is about $\delta \sim D/\sqrt{Re_p}$. A resolution of 5 cells in the boundary layer is expected to be sufficient [40] to resolve it accurately. Since the Prandtl number is 0.7, the momentum boundary layer and the thermal boundary layer have a similar thickness. This leads to a minimum cell size of $\Delta \leq D/50$ for $Re_p = 100$. This mesh requirement is confirmed by the mesh convergence study in Section 5.2. The final step in the workflow is to post-process the simulation results using a python script for Paraview [41].

To verify the solver, we performed numerical simulations of an isolated isothermal sphere in a uniform flow. We compared the calculated Nusselt number with the correlations of Whitaker [42] and Richter et al. [43]. We considered three Reynolds numbers (Re = 60, 120, 240) for a Prandtl number of 0.7. A uniform velocity and a constant fluid temperature of 530 K are specified at the inlet. The temperature of the sphere is fixed at 300 K. At the outlet and at

the side boundaries, the normal derivatives of temperature and velocity are set to zero. The domain size is $20D \times 10D \times 10D$, where *D* is the diameter of the sphere. The mesh size is $\Delta = D/20$. The center of the sphere is located at $(5D, 5D, 5D)_{x,y,z}$. Whitaker [42] proposed the following Nusselt number correlation for a single sphere:

$$Nu = 2 + \left(0.4Re^{0.5} + 0.06Re^{\frac{2}{3}}\right)Pr^{0.4}$$
(13)

Richter et al. [43] proposed a Nusselt number correlation extracted from simulation results with ANSYS FLUENT:

$$Nu = 1.76 + 0.55Pr^{1/3}Re^{0.5} + 0.014Pr^{1/3}Re^{2/3}$$
(14)

Fig. 3 compares the results of the current simulations with the correlation of Whitaker [42] and Richter et al. [43]. Good agreement is found between our results and the Whitaker correlation. The Nusselt numbers predicted by Richer et al. [43] are slightly higher than ours. The same finding was reported by Chen et al. [27] for a Prandtl number of 0.744.



Fig. 3 Nusselt numbers for a single sphere in a uniform flow as a function of the Reynolds number

4. Upscaling gas-solid heat transfer

The upscaling framework relies on the volume averaging process. Gas-solid heat transfer is modeled by convective flow between the filtered gas and solid temperatures. These temperatures are the resolved temperatures in a two-temperature model. The convective coefficient is evaluated by a Nusselt number correlation. Correct extraction of the correlation from the pore-scale simulation requires defining a statistical surface filter.

4.1. Volume average of the steady-state fluid energy equation

The REV is used as a spatial cut-off filter. Volume averaging over this volume allows the flow to be described with the average temperatures of the phases. These average temperatures are the filtered temperatures in the volume averaging method [16]. The detail of the subgrid geometry is no longer available. Therefore, each phase is considered as a continuous phase. Using the standard form of the spatial averaging operator, the volume average of any fluid function ψ_f is written:

$$\langle \psi_f \rangle = \frac{1}{V} \int_{V_f} \psi_f dV \tag{15}$$

where V_f represents the volume of the fluid phase and V the global volume. In addition, the intrinsic average can be defined as:

$$\langle \psi_f \rangle^f = \frac{1}{V_f} \int_{V_f} \psi_f dV \tag{16}$$

The superficial and intrinsic averages are related by the fluid volume fraction $\varepsilon_f = V_f / V$:

$$\langle \psi_f \rangle = \varepsilon_f \langle \psi_f \rangle^f \tag{17}$$

We also introduce the decomposition given by Gray [44]:

$$\psi_f = \langle \psi_f \rangle^f + \widetilde{\psi_f} \tag{18}$$

We apply the spatial averaging operator to the solved steady state fluid energy equation (1). Using the averaging theorem [45] which is a spatial form of the Leibniz integral rule, the filtered equation is written as follows:

$$\nabla \cdot \langle \boldsymbol{u}T_f \rangle + \frac{1}{V} \int_{A_{sf}} (\boldsymbol{u}T_f) \cdot d\boldsymbol{A} = a_f \nabla \cdot \langle \nabla T_f \rangle + \frac{a_f}{V} \int_{A_{sf}} \nabla T_f \cdot d\boldsymbol{A}$$
(19)

 $a_f = k_f / (\rho_f C_{p_f})$ is the thermal diffusivity and A_{sf} is the solid-fluid surface interface.

In the case of a fixed assembly, the velocity at solid-fluid interface is zero which leads to:

$$\nabla \cdot \langle \boldsymbol{u}T_f \rangle = a_f \nabla \cdot \langle \nabla T_f \rangle + \frac{a_f}{V} \int_{A_{sf}} \nabla T_f \cdot d\boldsymbol{A}$$
⁽²⁰⁾

Using Gray's decomposition, equation (20) writes:

$$\nabla \cdot \langle \boldsymbol{u}T_f \rangle = a_f \nabla \cdot \langle \nabla T_f \rangle + \frac{a_f}{V} \int_{A_{sf}} \langle \nabla T_f \rangle^f \cdot d\boldsymbol{A} + \frac{a_f}{V} \int_{A_{sf}} \widetilde{\mathcal{V}T_f} \cdot d\boldsymbol{A}$$
(21)

According to [16], equation (21) can be simplified as follows:

$$\nabla \cdot \langle \boldsymbol{u}T_f \rangle = a_f \nabla \cdot \langle \nabla T_f \rangle - a_f \nabla \varepsilon_f \langle \nabla T_f \rangle^f + \frac{a_f}{V} \int_{A_{sf}} \widetilde{\nabla T_f} \cdot d\boldsymbol{A}$$
(22)

Assuming no porosity gradient, i.e. $\nabla \varepsilon_f = 0$, equation (22) writes:

$$\nabla \cdot \langle \boldsymbol{u}T_f \rangle = a_f \nabla \cdot \langle \nabla T_f \rangle + \frac{a_f}{V} \int_{A_{sf}} \widetilde{VT_f} \cdot d\boldsymbol{A}$$
(23)

However, the evaluate of the divergence of the volume averaged value requires the use of several contiguous representative elementary volumes. To overcome this problem, we define a statistical surface filter in the Section 4.2. Thus, the differential operator of the filtered variable can be defined on a single REV.

4.2. Statistical surface filter

Fig. 4 shows a cross-section of the REV through YZ plane. The global area of the crosssection is $A = L \times L$. The global area A is the sum of the solid area and the fluid area noted A_f .

Fig. 4 Cross-section of the REV through YZ plane at x

Unlike the global area, the fluid area depends on the x location. Moreover, for several packing realizations at the same x position, the fluid area is not necessarily the same. Then, the fluid area is a function of the ω realization and the x position $A_f(\omega, x)$. Nevertheless, as pointed out by [23], the average over several realizations of the ratio of the global area to the fluid area converges to the fluid porosity. Indeed, the fluid porosity corresponds to the probability of fluid presence. This is expressed by equation (24) where *N* is the number of realizations.

$$\overline{1} = \frac{1}{N} \sum_{\omega=0}^{\omega=N} \frac{1}{A} \int_{A_f} 1 dA = \varepsilon_f \qquad \forall x$$
(24)

where the statistical surface filter is defined as:

$$\overline{\psi_f}(x) = \frac{1}{N} \sum_{\omega=0}^{\omega=N} \frac{1}{A} \int_{A_f} \psi_f(\omega) dA$$
(25)

Recalling that the probability of fluid presence can be expressed by the volume filter as follows:

$$\langle 1 \rangle = \frac{1}{V} \int_{V_f} 1 dV = \varepsilon_f \tag{26}$$

The statistical surface filter and the volume filter follow a form of ergodicity. The ensemble average of the surface filter is equivalent to the ensemble average of a REV. The filtered values can be considered equal.

We define the following decomposition:

$$\psi_f(x, y, z) = \overline{\psi_f}(x) + \widetilde{\psi_f}(x, y, z)$$
(27)

4.3. Statistical surface filtering of the steady-state fluid energy equation

The demonstration of the spatial averaging theorem is based on the Leibniz's rule. The proof in [16] can be extend to our surface average case. We use the same approach. Let us define s as the distance along any line included in a porous media cross-section illustrated in **Fig. 5** and ψ_f as a fluid function.





Fig. 5 Averaging surface in a porous media cross-section

We consider the following derivative:



Fig. 6 Differential displacement of the averaging surface

Defining τ as a unit vector tangent to the line included in the cross-section, then,

$$\frac{d}{ds} = \boldsymbol{\tau} \cdot \boldsymbol{\nabla} \tag{29}$$

We can define the variation of the surface as:

$$\frac{dA}{ds} = \boldsymbol{\tau} \cdot \frac{\nabla A}{\|\nabla A\|} \|\nabla A\| = \boldsymbol{\tau} \cdot \boldsymbol{n}_{fe} \, dl \tag{30}$$

$$\Delta A = \boldsymbol{\tau} \cdot \boldsymbol{n}_{fe} \, dl \, \Delta s \tag{31}$$

 n_{fe} is the unit normal of the surface boundary as shown in Fig. 5. Fig. 6 shows the two averaging surfaces A(s) and $A(s + \Delta s)$. The intersection of $A_f(s + \Delta s)$ and $A_f(s)$ in equation (28) can be remove. Then, the no-overlapping area is provided by equation (31). Therefore, we replace the surface integral by a linear integral:

$$\frac{d}{ds} \int_{A_f} \psi_f \, dA = \int_{\Gamma_{fe}} \boldsymbol{\tau} \cdot \boldsymbol{n}_{fe} \, \psi_f \, dl \tag{32}$$

 Γ_{fe} is the surface boundary illustrated in Fig. 5. Using the equation (29), equation (32) writes:

$$\nabla \int_{A_f} \psi_f \, dA = \int_{\Gamma_{fe}} \boldsymbol{n}_{fe} \, \psi_f \, dl \tag{33}$$

The closed fluid surface boundary is composed of a fluid to fluid boundary and a fluid to solid boundary. Integrate a fluid variable ψ_f on the surface boundary Γ_{fe} corresponds to integrate the variable on the fluid to fluid boundary as ψ_f is zero inside the solid. The fluid to solid boundary is Γ_{fs} with a normal vector \mathbf{n}_{fs} as depicted in **Fig. 5**. According to the defined closed fluid surface, we use the 2D divergence theorem to express the right-hand side of the equation (33) as:

$$\int_{\Gamma_{fe}} \boldsymbol{n}_{fe} \,\psi_f \, dl \,= \int_{A_f} \nabla \psi_f \, dA - \int_{\Gamma_{fs}} \boldsymbol{n}_{fs} \,\psi_f \, dl \tag{34}$$

Then, equation 33 can be write:

$$\nabla \int_{A_f} \psi_f \, dA = \int_{A_f} \nabla \psi_f \, dl \, - \int_{\Gamma_{sf}} \mathbf{n}_{fs} \, \psi_f \, dl \tag{35}$$

Using the filter notation, we find the classical form of the spatial averaging theorem, derived here for our statistical surface filter, with $dl = n_{fs} dl$:

$$\overline{\nabla \psi_f} = \nabla \overline{\psi_f} + \int_{\Gamma_{sf}} \psi_f dl$$
(36)

Therefore, applying the statistical surface filter to the fluid energy equation leads to:

$$\nabla \cdot \overline{\boldsymbol{u}}\overline{T_f} = a_f \nabla \cdot \overline{\nabla}\overline{T_f} + \frac{a_f}{A} \int_{\Gamma_{sf}} \widetilde{\nabla}\overline{T_f} \cdot d\boldsymbol{l}$$
(37)

The statistical surface filtered variables are a function of the single variable x, then, the equation (37) writes:

$$\frac{d\overline{u_xT_f}}{dx} = a_f \frac{d\overline{\nabla_xT_f}}{dx} + \frac{a_f}{A} \int_{\Gamma_{sf}} \widetilde{\nabla T_f} \cdot d\boldsymbol{l}$$
(38)

Using the mixing-cup temperature definition:

$$T_m = \frac{\overline{u_x T_f}}{\overline{u_x}} \tag{39}$$

$$\frac{dT_m}{dx} = \underbrace{\frac{a_f}{\overline{u_x}} \frac{d\overline{\nabla_x T_f}}{dx}}_{(1) mean \ axial \ conduction}} + \underbrace{\frac{a_f}{A\overline{u_x}} \int_{\Gamma_{sf}} \widetilde{\nabla T_f} \cdot dl}_{(2) \ aas-solid \ heat \ transfer}$$
(40)

The equation (40) contains two unclosed terms: (1) the mean axial conduction and (2) the gassolid heat transfer. We need to neglect the mean axial condition to compute gas-solid heat transfer term from the streamwise evolution of the mixing-cup temperature. The condition requires to neglect mean axial condition term is expressed in the section 4.4.

4.4. Condition to neglect mean axial conduction

We proceed to an adimensional scaling of the equation (40), defining:

$$T_m^* = \frac{T_m}{T_{m,i}} \qquad \overline{\nabla T_f}^* = \frac{\int_{\Gamma_{sf}} \overline{\nabla T_f} \cdot dl}{\left(\frac{\overline{T_f(0)} - \overline{T_f(L)}}{L}\right)P} \qquad \overline{\nabla_x T_f}^* = \frac{\overline{\nabla_x T_f}}{\left(\frac{\overline{T_f(0)} - \overline{T_f(L)}}{L}\right)}$$
(41)

P is the perimeter of the gas-solid interface in the cross-section. Then, the equation (40) becomes:

$$\frac{dT_m^*}{dx} = \frac{a_f}{\overline{u_x}} \frac{\overline{T_f(0)} - \overline{T_f(L)}}{L} \frac{d(\overline{\nabla_x T_f^*})}{dx} + \frac{a_f}{\overline{u_x}} \frac{\overline{T_f(0)} - \overline{T_f(L)}}{L} \frac{P}{A} \overline{V} \overline{T_f^*}$$
(42)

The mean axial conduction can be negleted if P/A >> 1, and according to [22]:

$$\frac{P}{A} = \frac{6\pi\varepsilon_s}{4D} \gg 1 \tag{43}$$

The condition (43) states that the gas-solid heat transfer is dominant in equation (40), as long as the REV describes a porous medium, i.e. a fluid volume containing several solid inclusions. Then, the interface perimeter is larger than the total surface area.

4.5. Evaluating Nusselt numbers to model pore-scale gas-solid heat transfer

Neglecting the mean axial conduction, the filtered fluid energy equation (40) writes:

$$\frac{dT_m}{dx} = \frac{a_f}{A\overline{u_x}} \int_{\Gamma_{sf}} \widetilde{\nabla T_f} \cdot dl$$
(44)

Following the heuristic approach, we modeled the integral term as a convective flux, with a convective coefficient h_m :

$$k_f \int_{\Gamma_{sf}} \widetilde{\nabla T_f} \cdot d\mathbf{l} = -h_m P(T_m - T_s)$$
(45)

Then, the equation (44) writes:

$$\frac{dT_m}{dx} = -\frac{Nu_m P}{Pe} \frac{P}{A} (T_m - T_s)$$
(46)

 $Pe = \overline{u_x}D/a_f$ is the Peclet number and $Nu_m = h_m D/k_f$ is the Nusselt number where the convective coefficient is based on the mixing cup temperature. However, as pointed out by [22], in a two-temperature model, the Nusselt number must be defined with the filtered temperature. Indeed, these are the solved temperatures. Equation (46) can be written in terms of filtered temperature, using the filtering rules:

$$\frac{d\overline{T}_{f}^{f}}{dx} = -\frac{Nu}{Pe}\frac{P}{A}\left(\overline{T}_{f}^{f} - T_{s}\right) - \underbrace{\frac{d\frac{\widetilde{u_{x}}\widetilde{T}}{\overline{u_{x}}}}{dx}}_{thermal \ dispersion}$$
(47)

 $Nu = hD/k_f$ is the Nusselt number defined in terms of the filtered temperature. The evolution of the filtered temperature in the flow direction depends on the thermal dispersion. Thus, heat transfer is not the only force driving the evolution of the filtered temperature. Thermal dispersion must therefore be expressed in terms of modeled convective flow to allow the derivation of the Nusselt number. This is done in [22] for the thermal ratio boundary condition. Instead, the proposed thermal offset boundary condition, section 3.2, imposes an equality of fluctuations along the streamwise direction, thus:

$$\frac{d\overline{\widetilde{\frac{u_x}\widetilde{T}}{u_x}}}{dx} = 0$$
(48)

Then,

$$\frac{d\overline{T_f}^{\,f}}{dx} = -\frac{Nu}{Pe}\frac{P}{A}\left(\overline{T_f}^{\,f} - T_s\right) \tag{49}$$

So, the Nusselt numbers can be evaluated as:

$$Nu_m = \frac{1}{N} \frac{1}{N_{slice}} \sum_{\omega=0}^{\omega=N} \sum_{x=0}^{x=L} \frac{D \int_0^{\Gamma_{sf}} \overline{\mathcal{V}T} \cdot d\boldsymbol{l}}{P(T_m - T_s)}$$
(50)

$$Nu = \frac{1}{N} \frac{1}{N_{slice}} \sum_{\omega=0}^{\omega=N} \sum_{x=0}^{x=L} \frac{D \int_0^{\Gamma_{sf}} \widetilde{VT} \cdot dl}{P(\overline{T_f}^f - T_s)}$$
(51)

 N_{slice} is the number of cross-section which is 250 for each realization ω .

5. Results

The proposed upscaling method is based on the extraction of Nusselt numbers using a statistical surface filter applied to pore-scale simulations. First, we verify that the thermal offset boundary condition expressed in Section 3.2 leads to a statistically quasi-homogeneous Nusselt number in the streamwise direction. Second, we establish the mesh convergence of the Nusselt number value extracted from a packing realization simulation. We also establish the statistical convergence of the Nusselt number extracted from several packing realizations. Finally, we discuss the global flow characteristics and correlations of the Nusselt number.

5.1. Streamwise Nusselt number behavior

As pointed out by [23], the Nusselt number should be statistically homogeneous. Then, in the equations (46) and (49), the Nusselt number is a constant. Fig. 7 shows the variation of the average Nusselt number (equation (51)) with the streamwise direction for 5 realizations of packing with $\varepsilon_f = 0.8$ for Re_p = 10 (Fig. 7 (a)) and Re_p = 100 (Fig. 7 (b)). On the first six sections, the average value of the Nusselt number is higher than on the other sections. The average Nusselt number from 5 realizations shows some variation along the streamwise direction. As pointed out by [23], this is due to the small number of realizations.



Fig. 7 Variation of the average Nusselt number in the streamwise direction. Symbols indicate average Nusselt number and error bars indicate 95% confidence intervals [46]. Only 125 cross-sections are shown for better visualization. (a) $Re_p = 10 \epsilon_f = 0.8$ for 5 realizations (b) $Re_p = 100 \epsilon_f = 0.8$ for 5 realizations

By increasing the number of realizations to 18, the average Nusselt number is almost constant along the streamwise direction as shown on **Fig. 8**. However, the higher average Nusselt number over the first 6 cross-sections remains. Still, the relative error introduces by the 6 cross-sections, estimated from present results, is about 2%. The Nusselt number can be considered as constant and the equation (50) and (51) can be used.



Fig. 8 Variation of the average Nusselt number in the streamwise direction. Symbols indicate average Nusselt number and error bars indicate 95% confidence intervals [46]. $Re_p = 10 \ \varepsilon_f = 0.8$ for 18 realizations

5.2. Mesh convergence

We used uniform grid resolution $\Delta x = \Delta y = \Delta z$. We performed several simulations with different grid resolutions on the same packing for the same Reynolds number ($\varepsilon_f = 0.8$ and Re_p = 100). Fig. 9 (a) shows the convergence of the Nusselt number based on mixing-cup temperature. Fig. 9 (b) shows the convergence of the Nusselt number based on filtered temperature. Both Nusselt numbers converge to an asymptotic value starting at $D/\Delta x = 50$. The relative error between the coarsest grid and the finest one is about 8% and 5% for Nu_m and Nu respectively. Therefore, all simulations in Table 1 are performed with grid resolution $D/\Delta x = 50$.



Fig. 9 (a) Nusselt number based on mixing-cup temperature convergence with grid resolution for $\varepsilon_f = 0.8 \ Re_p = 100. \ D/\Delta x$ is the sphere diameter over the grid size. (b) Nusselt number based on filtered temperature convergence with grid resolution for $\varepsilon_f = 0.8 \ Re_p = 100$.

5.3. Average convergence

We performed several packing configurations (ω) for Re_p = 10 and $\varepsilon_f = 0.8$ with the grid resolution $D/\Delta x = 50$. Fig. 10 shows the statistical convergence of the average Nusselt

number for mixing-cup temperature and filtered temperature. The convergence is achieved with 35 configurations. The confidence interval is calculated using the Student's t-distribution [46]. The confidence interval decreases sharply between 5 and 15 configurations. Therefore, we choose a compromise between accuracy and number of simulations, namely 8 configurations.



Fig. 10 (a) Nusselt number based on the mixing-cup temperature statistical convergence, i.e. with the number of configurations, for the case $Re_p = 10 \ \varepsilon_f = 0.8$. (b) Nusselt number based on the filtered temperature statistical convergence for the case $Re_p = 10 \ \varepsilon_f = 0.8$. Square symbols indicate average Nusselt number and error bars indicate 95% confidence intervals.

5.4. Global temperature and velocity field

Fig. 11 shows the evolution of the scaled temperature defined as:

$$T_{scale} = \frac{T_f - T_s}{T_{m,i} - T_s} \tag{52}$$

The temperature field shows similar behavior for the different Reynolds numbers considered. However, for $Re_p = 20$, the temperature decreases quickly with the axial coordinate. The fluidsolid system approaches equilibrium. As shown in [23], for $\varepsilon_f < 0.6$ and $Re_p < 10$ the average fluid temperature decays over a particle diameter. For these systems, other closure method for the gas-solid heat transfer should be used.



Fig. 11 Scaled temperature evolution in a cross-section plane for $\varepsilon_f = 0.6$ at several Reynolds number (a) $Re_p = 20$ (b) $Re_p = 50$ (c) $Re_p = 100$ (in color)

As shown by the scaled velocity norm $(||U_{scale}|| = ||u||/Re_p)$ field in Fig. 12, the flow structure remains essentially the same for these Reynolds numbers. For higher Reynolds numbers, smaller length scales can be noticed on the velocity norm. This can be clearly seen by observing the change between Reynolds numbers in the lower right corner of the figures.



Fig. 12 Scaled velocity norm field in a transversal plane for $\varepsilon_f = 0.6$ at several Reynolds number (a) $Re_p = 20$ (b) $Re_p = 50$ (c) $Re_n = 100$ (in color)

5.5. Nusselt number based on the mixing-cup temperature

A widely used Nusselt number correlation for modeling heat transfer in packed beds is the Gunn correlation. This correlation was derived from four asymptotic relationships and experimental evidence for the dependence of the Nusselt number on porosity. The analysis is based on statistical properties of the flow. The fixed bed is considered as an assembly of flow channels. Each flow channel has a central point, and a radial vector of length η can be defined from this point. The fluid surface distribution is a function of η . Then, the statistical presence of the flow surface is introduced by a probability density distribution. This probability density function is independent of the streamwise coordinate. The heat transport equation is then written in the streamwise and the radial coordinates. Considering that the pore scale convection term can be decomposed as follows:

$$\frac{1}{\overline{u_x}}\frac{\partial u_x T}{\partial x} = \frac{dT_m}{dx} + \underbrace{\frac{d\frac{u_x T}{\overline{u_x}}}{dx}}_{therm \ mixing}$$
(53)

Since the probability density function of fluid area does not depend on the coordinate in the streamwise direction, thermal mixing does not occur in this direction. For the thermal offset boundary condition, the thermal mixing term is also zero. Therefore, our pore-scale simulation leads to the same prediction of the temperature evolution of the mixing cup. Therefore, we expect similar results between the Gunn correlation prediction and our extracted Nusselt number. The correlation of the Gunn's Nusselt number is written as follows:

$$Nu_m = \left(7 - 10\varepsilon_f + 5\varepsilon_f^2\right) \left(1 + 0.7Re^{0.2}Pr^{\frac{1}{3}}\right) + (1.33 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)Re_p^{0.7}Pr^{\frac{1}{3}}$$
(54)

Fig. 13 shows the comparison between the Nusselt number derived from the pore-scale simulations and the Gunn correlation. As expected, a very good agreement is found between both. This demonstrates, as a validation, the ability of the new upscaling framework to reproduce well-known results for sphere packings.



Fig. 13 Dependency of the Nusselt number based on mixing-cup temperature on the Reynolds number. The symbols are the pore-scale simulations results and the error bars indicate 95% confidence intervals. The lines are obtained from Gunn's correlation.

The results obtained in [22] use the thermal ratio boundary condition expressed in section 3.2, instead of the proposed thermal offset boundary condition. For thermal ratio boundary condition, the thermal mixing (equation 53) evolution is not zero. Therefore, the mixing-cup temperature evolution has a smaller value than for the thermal offset boundary condition and for the Gunn's analysis. Thus, the Nusselt number (Nu_m) calculated with the thermal ratio boundary condition. The correlation of Sun writes:

$$Nu_m = \left(-0.46 + 1.77\varepsilon_f + 0.69\varepsilon_f^2\right)/\varepsilon_f^3 + (1.37 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)Re_p^{0.7}Pr^{\frac{1}{3}}$$
(55)

Fig. 14 shows the comparison between the Nusselt number extracted from the current porescale simulation with the Gunn correlation, Sun correlation, and PR-DNS results. As expected, the Nusselt number based on mixing-cup temperature predicted in [22] is lower than that of the Gunn correlation or our results. Both thermal boundary conditions respect the introduction of a constant energy flux in the pore-scale simulation. However, the thermal ratio condition introduces a thermal mixing effect on the mixing-cup temperature.



Fig. 14 Dependency of the Nusselt number based on mixing-cup temperature on the Reynolds number. The triangle symbols are the pore-scale results and the error bars indicate 95% confidence intervals. The circle symbols are the data from Sun et al. [22]. The lines are obtained from the Sun and the Gunn correlations

5.6. Nusselt number based on the filtered temperature

Sun's correlation for the Nusselt number based on the mixing-cup temperature can be derived for the Nusselt number based on the filtered temperature. This is done by using the correlation of the average scaled fluid temperature from [22]:

$$Nu = \frac{\left(-0.46 + 1.77\varepsilon_f + 0.69\varepsilon_f^2\right)/\varepsilon_f^3 + (1.37 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)Re_p^{0.7}Pr^{\frac{1}{3}}}{1 - 1.6\varepsilon_s\varepsilon_f - 3\varepsilon_s\varepsilon_f^4\exp\left(-Re_p^{0.4}\varepsilon_s\right)}$$
(56)

Considering the filtering rules and equation (47):

$$\frac{dT_m}{dx} = \frac{d\overline{T_f}^f}{dx} + \underbrace{\frac{d\overline{u_x}\tilde{T}}{u_x}}_{therm \ dispersion} = -\frac{Nu}{Pe} \frac{P}{A} \left(\overline{T_f}^f - T_s\right)$$
(57)

For both thermal (offset or ratio) boundary condition, the Nusselt number does not depend on the streamwise location. Therefore, the inhomogeneity in the mixing-cup temperature arises solely from the inhomogeneity of the filtered temperature.

According to [22], the thermal ratio boundary condition leads to a statistically homogeneous scaled fluid temperature:

$$\frac{d\bar{\theta}}{dx} = \frac{d}{dx} \left(\frac{\bar{T}_f^{\ f} - T_s}{T_m - T_s} \right) = 0 \tag{58}$$

Then,

$$\frac{dT_m}{dx} = \frac{1}{\bar{\theta}} \frac{d\bar{T}_f^{\ f}}{dx}$$
(59)

Introducing equation (59) in equation (57) leads to:

$$\frac{d\frac{\widetilde{u_x}\widetilde{T}}{\overline{u_x}}}{dx} = \frac{(1-\overline{\theta})}{\overline{\theta}}\frac{d\overline{T_f}^f}{dx}$$
(60)

The thermal ratio boundary condition enforces a relationship between the thermal dispersion and the evolution of the filtering temperature. Then, equation (57) can be write in terms of the evolution of the filtered temperature:

$$\frac{d\overline{T}_{f}^{\ f}}{dx} = -\overline{\theta} \frac{Nu}{Pe} \frac{P}{A} \left(\overline{T}_{f}^{\ f} - T_{s}\right)$$
(61)

For the present offset boundary condition, the thermal dispersion is zero. Then, the evolution of the filtering temperature writes:

$$\frac{d\overline{T}_{f}^{\ f}}{dx} = -\frac{Nu}{Pe}\frac{P}{A}\left(\overline{T}_{f}^{\ f} - T_{s}\right)$$
(62)

The solutions to equation (61) and (62) write respectively, with $\alpha = P/(PeA)$:

$$\varphi_{sun} = \frac{\overline{T_f}^f - T_s}{\overline{T_f}^f(0) - T_s} = e^{-\alpha \overline{\theta} N u x}$$
(63)

$$\varphi_{present} = \frac{\overline{T_f}^T - T_s}{\overline{T_f}^f(0) - T_s} = e^{-\alpha N u x}$$
(64)



Fig. 15 Evolution of the non-dimensional filtered temperature in the streamwise direction for $\varepsilon_f = 0.6 Re_p = 100$. Lines are the exponential models. Triangle symbols are the Sun et al. [35] results and circle are present results.

Fig. 15 shows the evolution of the non-dimensional filtered temperature for thermal ratio (Sun et al. results) and thermal offset boundary condition (present results), as well as the corresponding exponential model. The thermal ratio boundary condition leads to a lower exponential decay of the non-dimensional filtered value. This is due to the thermal dispersion term which is non-zero in this case. The thermal dispersion reduces the temperature gradient, which reduces the heat transfer. Therefore, the decay of the non-dimensional filtered value is lower. However, since the inhomogeneity in the mixing-cup temperature arises solely from the inhomogeneity of the filtered temperature, and the thermal dispersion is related to the filtered temperature both thermal conditions lead to the same prediction of the Nusselt number. Fig. 16 shows Sun's correlation extended to higher solid volume fractions $\varepsilon_s > 0.5$ and compared to our pore-scale results. Very good agreement is found between the Sun correlation and our results, even for the extended part.



Fig. 16 Dependency of the Nusselt number based on filtered temperature on the Reynolds number. The symbols are the porescale results and the error bars indicate 95% confidence intervals. The lines are obtained from Sun's correlation which is extended here to cases where $\varepsilon_s > 0.5$.

6. Discussions

Several authors [47] [48] [28] [22] who derived Nusselt number from pore-scale simulations have claimed that the Gunn model overestimates the Nusselt number. However, our work shows that we must distinguish the Nusselt number calculated based on the mixing-cup temperature, Nu_m , from that calculated based on the filtered temperature, Nu. The Nusselt number calculated based on the filtered temperature is the only valid number to use with the filtered temperature in the two-temperature model. As highlighted in this work, Nu_m values extracted from the pore-scale simulations depend on the velocity and temperature boundary conditions. This is the reason for the observed differences between Gunn's correlation and the correlations extracted from other work. Using Gunn's Nusselt number correlation for two-temperature model leads to the evaluation of Nu_m which, according to our results and those of Sun et al. [22], is lower than the valid Nu to be used with the filtered temperature. Fig. 17 shows the comparison of the dependence of Nu_m and Nu on the Reynolds number. Nu_m is weaker than Nu. Furthermore, this behavior is more pronounced as the solid volume fraction ε_s increases.

Thus, using the Nusselt number from the Gunn correlation in a two-temperature model leads to an underestimation of the heat transfer between phases.



Fig. 17 Comparison between the Nusselt number based on filtered temperature Nu from the Sun et al. [22] correlation extended to case $\varepsilon_s > 0.5$ and the Nusselt number based on the mixing-cup temperature Nu_m from the Gunn's correlation.

In case of fluidized beds, the movement of the particles carrying their temperature should modifies the evolution of the filtered temperature. One way to take this phenomenon into account would probably be to introduce a statistical treatment of the particles motion. Nevertheless, as reported in [22], there is no mean velocity gradient in the hydrodynamic problem. This suggests that in a statistical sense, the particle motion would have no impact on the evolution of the filtered temperature.

This work proposes an evaluation method for the Schuman two-temperature model [15]:

$$\frac{\partial \langle T_f \rangle^f}{\partial t} + \nabla \cdot \left(\langle \boldsymbol{u} \rangle^f \langle T_f \rangle^f \right) = -\frac{N u \, a_f A_{sf}}{D \, V_f} \left(\langle T_f \rangle^f - T_s \right) \tag{65}$$

$$\frac{\partial \langle T_s \rangle^s}{\partial t} = \frac{Nu \, a_s A_{sf}}{D \, V_s} \left(\langle T_f \rangle^f - T_s \right) \tag{66}$$

For sphere packing, the Nusselt number can be evaluated with the Sun correlation (equation 56). The present work has shown that this correlation can be extended to dense sphere packings. However, the proposed upscaling framework is not limited to sphere packing. The method can be used to evaluate Nusselt number for other types of assembly.

It should be noted that the mean conduction is neglected as suggested by the adimensional scaling in Section 4.4. We recall that the fluid mean conduction writes as follows:

$$a_{f}\nabla \cdot \langle \nabla T_{f} \rangle^{f} = \underbrace{a_{f} \nabla^{2} \langle T_{f} \rangle^{f}}_{(diffusion)} + \underbrace{\frac{a_{f}}{V_{f}} \nabla \cdot \int_{A_{sf}} \widehat{T_{f}} \cdot dA}_{(tortuosity)}$$
(67)

Then, neglecting fluid mean conduction leads to neglect diffusion and tortuosity terms as defined by D'Hueppe [10]. We assume that the same hypotheses can be done for solid mean conductivity. The current upscaling framework is restricted to cases where solid thermal response is much larger than fluid thermal response. This is usually the case for gas-solid flow. However, for high pressure, the fluid thermal response can increase significantly. In this case, a correct description would involve a coupled solution. However, these unsteady simulations are expected to be quite computationally expensive.

7. Conclusions

A new upscaling framework was derived to evaluate the Nusselt number from pore-scale simulations of gas-solid heat transfer in a packed bed. A robust thermal boundary condition of heat offset was developed to achieve Nusselt number evaluation even for high solid volume fractions $\varepsilon_s > 0.5$. The distinction between Nusselt number based on mixing-cup temperature and filtered temperature was explained. Hence, we have shown that the valid Nusselt number to be used with the two-temperature model is the Nusselt number based on the filtered temperature. The result of the pore-scale simulations for the mixing-cup Nusselt number shows good agreement with the Gunn correlation. In addition, the results for filtered temperature Nusselt number show good agreement with the Sun correlation. For comparison purpose the Sun correlation behavior is the same as the present results. This demonstrates the validity of the Sun's correlation for higher solid porosity. Thus, the upscaling method has been successfully applied to sphere packings and can be applied to other types of assemblies. This result has practical application to improve the evaluation $\varepsilon_s \cong 0.6$.

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