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An equation for thermal dispersion flux transport and its mathematical modelling for heat and fluid flow in a porous medium

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It is shown for the first time that the gradient diffusion hypothesis often adopted for thermal dispersion heat flux in heat transfer within porous media can be derived from a transport equation for the thermal dispersion heat flux based on the Navier–Stokes and energy equations. The transport equation valid for both thermal equilibrium and non-equilibrium cases is mathematically modelled so that all unknown spatial correlation terms, associated with redistribution and dissipation of the dispersion heat flux, are expressed in terms of determinable variables. The unknown coefficients are determined analytically by considering of macroscopically unidirectional flow through a tube as treated by Taylor. Taylor's expression for the dispersion has been generated from the transport equation. Both laminar and turbulent flow cases are investigated to obtain two distinct limiting expressions for low- and high-Péclet-number regimes. The results obtained for the Taylor diffusion problem are translated to the case of heat and fluid flow in a packed bed, to obtain the corresponding expressions for the axial dispersion coefficient in a packed bed. The resulting expression for the high-Péclet-number case agrees well with the empirical formula, validating of the present transport analysis.

1. Introduction

Dispersion is the spreading of mass or heat caused by variations in fluid velocity about the mean velocity. In addition to molecular thermal diffusion, there is significant mechanical dispersion in heat and fluid flow in a fluid-saturated porous medium, as a result of hydrodynamic mixing of the fluid particles passing through pores. This thermal dispersion causes additional heat transfer, which leads to complications in dealing with transport processes in fluid-saturated porous media.

Yagi, Kunii & Wakao (1960) and Wakao & Kaguei (1996) experimentally investigated the enhanced mixing due to mechanical dispersion. They assembled the results in terms of apparent axial and transverse conductivities, i.e. the dispersion coefficients. Their experimental data based on measurements of effective conductivities of packed beds revealed that the longitudinal dispersion coefficient is much larger than the transverse one. Following the initiative work by Yagi *et al.* (1960), a number of researchers conducted experimental investigations, such as Gunn & Khalid (1975), Li & Finlayson (1977) and Hunt & Tien (1988). An excellent review may be found in Vafai & Amiri (1998).

One of the simplest ways to illustrate the mechanism of thermal dispersion is to consider the rate of spreading of the heat (or mass) content caused by the radial

velocity non-uniformity of the fluid flowing inside a circular tube. This problem was considered by Taylor (1953) and later generalized by Aris (1956). The analytical expression for the effective diffusion coefficient based on the Taylor dispersion equation for sample concentration is used for various chromatographic measurement methodologies. Since this analytical treatment in a tube by Taylor, a number of theoretical and experimental efforts (e.g. Koch & Brady 1985; Han, Bhakta & Carbonell 1985; and Vortmeyer 1975) have been made to establish useful correlations for estimating the effective thermal conductivities due to thermal dispersion (see Kaviany 1995). Recently, Golfier, Quintard & Whitaker (2002) have appealed to a volume-averaging theory with a two medium treatment and predicted an axial dispersion coefficient which is somewhat less than Taylor's. Fried & Combornous (1971) and Kaviany (1995) provided excellent reviews on the Taylor–Aris dispersion problem and related matters.

In recent years, a series of numerical attempts have been made to determine the thermal dispersion coefficients directly from numerical experiments. Full Navier–Stokes and energy equations were solved by Eidsath *et al.* (1983) and Edwards *et al.* (1991) for flows through a periodic structure of circular cylinders with in-line and staggered arrangements. Arquis, Caltagirone & Le Breton (1991) extended the numerical model proposed by Coulaud, Morel & Caltagirone (1988) to the coupling of momentum and heat transfer to study both axial and transverse dispersion coefficients. The elegance of Arquis and his group is that they imposed a macroscopic temperature gradient either normal or parallel to a macroscopically uniform flow such that the microscopic temperature field within only one structural unit is needed, as in the velocity field, to determine the corresponding dispersion coefficient. Kuwahara, Nakayama & Koyama (1996) and Kuwahara & Nakayama (1999) followed the numerical approach proposed by Arquis *et al.*, assuming a macroscopically uniform flow through a lattice of rods, to elucidate the effects of microscopic velocity and temperature fields on the thermal dispersion. They set a macroscopically uniform flow passing through a lattice of square rods placed regularly in an infinite space, where a macroscopically linear temperature gradient was imposed either perpendicular or parallel to the flow direction. The macroscopic results were integrated over a unit structure to evaluate both transverse and longitudinal thermal dispersion coefficients. Two sets of distinct expressions for the transverse dispersion, as a function of the porosity and Péclet number, were established for the low- and high-Péclet-number ranges. This numerical experiment, which agrees well with available experiments, confirms that the longitudinal dispersion is substantially higher than the transverse dispersion, as reported by Yagi *et al.* (1960) who were the first to measure the effective longitudinal (axial) thermal conductivities of packed beds.

In all these previous investigations, gradient hypotheses were employed in which the dispersion heat flux is proportional to the gradient of the volume-averaged temperature with the proportionality coefficient being the dispersion thermal conductivity. Although available experimental and numerical data suggest the validity of such gradient hypotheses, its fundamental transport mechanism has never been examined in terms of the conservation equations based on first principles. To our knowledge, the transport equation of the dispersion heat flux vector based on first principles has never been explored to derive the expressions for the dispersion heat flux components. In this paper, we shall derive such a transport equation valid for both thermal equilibrium and non-equilibrium cases from the volume-averaged version of Navier–Stokes and energy equations, and perform mathematical modelling for the spatial correlation terms associated with redistribution and dissipation of the

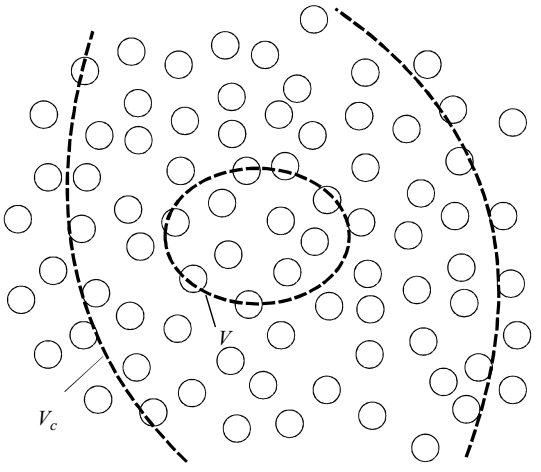

FIGURE 1. Microscopic view of porous structure.

dispersion heat flux. The unknown coefficients in the resulting model equation will be determined analytically by considering a homogeneous macroscopic flow through a bundle of circular tubes with microscopic velocity and temperature profiles as assumed by Taylor. Both laminar and turbulent flow cases will be treated, to obtain two distinct expressions, namely, low- and high-Péclet-number expressions for the dispersion thermal conductivities. The resulting expressions for the tube flow will be transformed to estimate the thermal dispersion in packed beds, upon appealing to an equivalent tube diameter concept.

2. Volume-averaged governing equations

In order for the volume averaging (smoothing process) to be meaningful, we consider a control volume V in a fluid-saturated porous medium, as shown in figure 1, whose length scale $V^{1/3}$ is much smaller than the macroscopic characteristic length $V_c^{1/3}$, but, at the same time, much greater than the microscopic (porous structure) characteristic length (see e.g. Nakayama 1995). Under this condition, the volume average of a certain variable ϕ is defined as

$$\langle \phi \rangle \equiv \frac{1}{V} \int_{V_f} \phi \, \mathrm{d}V. \tag{1}$$

Another average, namely, the intrinsic average, is given by

$$\langle \phi \rangle^f \equiv \frac{1}{V_f} \int_{V_f} \phi \, \mathrm{d}V \tag{2}$$

where V_f is the volume space which the fluid occupies. Obviously, the two averages are related as

$$\langle \phi \rangle = \varepsilon \langle \phi \rangle^f \tag{3}$$

where $\varepsilon \equiv V_f / V$ is the porosity. Following Cheng (1978), Quintard & Whitaker (1993), Nakayama (1995) and many others, we decompose a variable into its intrinsic average and the spatial deviation from it:

$$\phi = \langle \phi \rangle^f + \tilde{\phi}. \tag{4}$$

We shall exploit the following spatial average relationships:

$$\langle \phi_1 \phi_2 \rangle^f = \langle \phi_1 \rangle^f \langle \phi_2 \rangle^f + \langle \tilde{\phi}_1 \tilde{\phi}_2 \rangle^f, \tag{5}$$

$$\langle \nabla \phi \rangle = \nabla \langle \phi \rangle + \frac{1}{V} \int_{A_{\text{int}}} \phi \, \mathrm{d}\boldsymbol{A} \quad \text{or} \quad \langle \nabla \phi \rangle^f = \frac{1}{\varepsilon} \nabla \varepsilon \langle \phi \rangle^f + \frac{1}{V_f} \int_{A_{\text{int}}} \phi \, \mathrm{d}\boldsymbol{A}, \tag{6a, b}$$

and

$$\left\langle \frac{\partial \phi}{\partial t} \right\rangle = \frac{\partial \langle \phi \rangle}{\partial t} \tag{7}$$

where A_{int} is the local interface between the fluid and solid, while $\mathrm{d}\boldsymbol{A}$ is its vector element pointing outward from the fluid side to the solid side. The similarity between the volume averaging and the Reynolds averaging used in the study of turbulence is quite obvious. However, it should be noted that the present volume averaging procedure is somewhat more complex than the Reynolds averaging procedure, since it involves surface integrals, as clearly seen from (6).

We consider the microscopic governing equations, namely, the continuity equation, Navier–Stokes equation (with negligible body force) and energy equations (with negligible frictional heat generation under small Eckert number) for two phases:

$$\frac{\partial u_j}{\partial x_j} = 0, \tag{8}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} u_j u_i = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \nu_f \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \tag{9}$$

$$\rho_f c_{p_f} \left(\frac{\partial T}{\partial t} + \frac{\partial}{\partial x_j} u_j T \right) = \frac{\partial}{\partial x_j} \left(k_f \frac{\partial T}{\partial x_j} \right), \tag{10}$$

$$\rho_s c_s \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_j} \left(k_s \frac{\partial T}{\partial x_j} \right), \tag{11}$$

where the subscripts f and s stand for the fluid and solid, respectively, and ν_f is kinematic viscosity. It is assumed that the fluid is incompressible and all properties are constant. We consider a random rigid porous structure, and integrate spatially the foregoing microscopic governing equations, using the spatial average relationships given by (5) to (7). The resulting volume-averaged (macroscopic) governing equations are as follows:

$$\frac{\partial \langle u_j \rangle^f}{\partial x_j} = 0, \tag{12}$$

$$\frac{\partial \langle u_i \rangle^f}{\partial t} + \frac{\partial}{\partial x_j} \langle u_j \rangle^f \langle u_i \rangle^f = -\frac{1}{\rho_f} \frac{\partial \langle p \rangle^f}{\partial x_i} + \frac{\partial}{\partial x_j} \nu_f \left(\frac{\partial \langle u_i \rangle^f}{\partial x_j} + \frac{\partial \langle u_j \rangle^f}{\partial x_i} \right) + \frac{1}{V_f} \int_{A_{\text{int}}} \left(-\frac{p}{\rho} + \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) n_j \, \mathrm{d}A - \frac{\partial}{\partial x_j} \langle \tilde{u}_j \tilde{u}_i \rangle^f, \tag{13}$$

$$\varepsilon \rho_f c_{p_f} \left(\frac{\partial \langle T \rangle^f}{\partial t} + \frac{\partial}{\partial x_j} \langle u_j \rangle^f \langle T \rangle^f \right) = \frac{\partial}{\partial x_j} \left(\varepsilon k_f \frac{\partial \langle T \rangle^f}{\partial x_j} + \frac{k_f}{V} \int_{A_{\text{int}}} T n_j \, \mathrm{d}A - \varepsilon \rho_f c_{p_f} \langle \tilde{u}_j \tilde{T} \rangle^f \right) + \frac{1}{V} \int_{A_{\text{int}}} k_f \frac{\partial T}{\partial x_j} n_j \, \mathrm{d}A, \tag{14}$$

$$(1-\varepsilon)\,\rho_s c_s \frac{\partial \langle T\rangle^s}{\partial t} = \frac{\partial}{\partial x_j}\left((1-\varepsilon)\,k_s \frac{\partial \langle T\rangle^s}{\partial x_j} - \frac{k_s}{V}\int_{A_{\text{int}}} T n_j \,\mathrm{d}A\right) - \frac{1}{V}\int_{A_{\text{int}}} k_f \frac{\partial T}{\partial x_j} n_j \,\mathrm{d}A, \tag{15}$$

where $\langle T\rangle^s$ is the intrinsic average of the solid temperature, and n_j is the unit vector pointing outward from the fluid side to the solid side. The porosity ε is assumed to be constant within a medium. Moreover, the no-slip conditions are used over the interface of the rigid solid structure. Note that the dispersion heat flux $\rho_f c_{pf}\langle \tilde{u}_j \tilde{T}\rangle = \varepsilon \rho_f c_{pf}\langle \tilde{u}_j \tilde{T}\rangle^f$ appears in the volume-averaged energy equation (14) for the fluid phase.

In order to close the above macroscopic equations (12) to (15), the terms associated with the surface integral are modelled according to Vafai & Tien (1981) as

$$\frac{1}{V_f}\int_{A_{\text{int}}}\left(-\frac{p}{\rho_f} + \nu_f\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) n_j \,\mathrm{d}A - \frac{\partial}{\partial x_j}\langle \tilde{u}_j \tilde{u}_i\rangle^f = -\frac{\nu_f}{K}\varepsilon\langle u_i\rangle^f - b\varepsilon^2(\langle u_k\rangle^f \langle u_k\rangle^f)^{1/2}\langle u_i\rangle^f \tag{16}$$

which is the well-known Forchheimer-extended Darcy law, where K and b are the permeability and Forchheimer constant, respectively. The term describing the interfacial heat transfer between the fluid and solid, namely,

$$\frac{1}{V}\int_{A_{\text{int}}} k_f \frac{\partial T}{\partial x_j} n_j \,\mathrm{d}A = a_f h_f(\langle T\rangle^s - \langle T\rangle^f), \tag{17}$$

is modelled according to Newton's cooling law, where a_f and h_f are the specific surface area and interfacial heat transfer coefficient, respectively. Furthermore, the surface integral terms

$$\frac{k_f}{V}\int_{A_{\text{int}}} T n_j \,\mathrm{d}A \quad \text{and} \quad -\frac{k_s}{V}\int_{A_{\text{int}}} T n_j \,\mathrm{d}A$$

present the tortuosity heat fluxes, which are usually small as convection dominates over conduction (see e.g. Nakayama *et al.* 2001). Thus, the macroscopic momentum and energy equations may be written as

$$\frac{\partial \langle u_i\rangle^f}{\partial t} + \frac{\partial}{\partial x_j}\langle u_j\rangle^f \langle u_i\rangle^f = -\frac{1}{\rho}\frac{\partial \langle p\rangle^f}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f\left(\frac{\partial \langle u_i\rangle^f}{\partial x_j} + \frac{\partial \langle u_j\rangle^f}{\partial x_i}\right) - \frac{\nu_f}{K}\varepsilon\langle u_i\rangle^f - b\varepsilon^2(\langle u_k\rangle^f \langle u_k\rangle^f)^{1/2}\langle u_i\rangle^f, \tag{18}$$

$$\varepsilon\rho_f c_{p_f}\left(\frac{\partial \langle T\rangle^f}{\partial t} + \frac{\partial}{\partial x_j}\langle u_j\rangle^f \langle T\rangle^f\right) = \frac{\partial}{\partial x_j}\left(\varepsilon k_f \frac{\partial \langle T\rangle^f}{\partial x_j} - \varepsilon\rho_f c_{p_f}\langle \tilde{u}_j \tilde{T}\rangle^f\right) - a_f h_f(\langle T\rangle^f - \langle T\rangle^s), \tag{19}$$

$$(1-\varepsilon)\,\rho_s c_s \frac{\partial \langle T\rangle^s}{\partial t} = \frac{\partial}{\partial x_j}\left((1-\varepsilon)\,k_s \frac{\partial \langle T\rangle^s}{\partial x_j}\right) - a_s h_f(\langle T\rangle^s - \langle T\rangle^f). \tag{20}$$

For the cases of thermal equilibrium, namely, $\langle T\rangle^f = \langle T\rangle^s$, two energy equations are conveniently combined to form a single energy equation for the fluid-saturated porous media:

$$(\varepsilon\rho_f c_{p_f} + (1-\varepsilon)\,\rho_s c_s)\frac{\partial\langle T\rangle^f}{\partial t} + \varepsilon\rho_f c_{p_f}\frac{\partial}{\partial x_j}\langle u_j\rangle^f\langle T\rangle^f = \frac{\partial}{\partial x_j}\left((\varepsilon k_f + (1-\varepsilon)k_s)\frac{\partial\langle T\rangle^f}{\partial x_j} - \varepsilon\rho_f c_{p_f}\langle\tilde{u}_j\tilde{T}\rangle^f\right). \quad (21)$$

Thus, in the case of thermal equilibrium, we need only determine the dispersion heat flux $\rho c_{pf}\langle\tilde{u}_j\tilde{T}\rangle$. However, in what follows, we shall derive the transport equation for $\langle\tilde{u}_j\tilde{T}\rangle$ valid not only for the case of thermal equilibrium but also for the case of non-thermal equilibrium.

3. Dispersion heat flux transport equation

Having established the set of volume-averaged governing equations, we shall follow a procedure analogous to the one used in deriving the Reynolds stress transport equation. Thus, we first subtract the macroscopic equations (12), (18) and (19) from the microscopic equations (8), (9) and (10), respectively, and obtain the corresponding transport equations for the spatial deviations as follows:

$$\frac{\partial\tilde{u}_j}{\partial x_j} = 0, \quad (22)$$

$$\frac{\mathrm{D}\tilde{u}_i}{\mathrm{D}t} + \frac{\partial}{\partial x_j}(\tilde{u}_j\langle u_i\rangle^f + \tilde{u}_i\tilde{u}_j) = -\frac{1}{\rho_f}\frac{\partial\tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i}\right) + \frac{\nu_f}{K}\varepsilon\langle u_i\rangle^f + b\varepsilon^2(\langle u_k\rangle^f\langle u_k\rangle^f)^{1/2}\langle u_i\rangle^f, \quad (23)$$

$$\frac{\mathrm{D}\tilde{T}}{\mathrm{D}t} + \frac{\partial}{\partial x_j}(\tilde{u}_j\langle T\rangle^f + \tilde{u}_j\tilde{T} - \langle\tilde{u}_j\tilde{T}\rangle^f) = \frac{\partial}{\partial x_j}\left(\alpha_f\frac{\partial\tilde{T}}{\partial x_j}\right) + \frac{a_s h_f}{\varepsilon\rho_f c_{p_f}}(\langle T\rangle^f - \langle T\rangle^s), \quad (24)$$

where α_f is the thermal diffusivity of the fluid and

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} \equiv \frac{\partial\phi}{\partial t} + \langle u_j\rangle^f\frac{\partial\phi}{\partial x_j} \quad (25)$$

is a shorthand notation for the substantial derivative based on the intrinsic velocity. We note the obvious relationship

$$\frac{\mathrm{D}\tilde{u}_i\tilde{T}}{\mathrm{D}t} = \tilde{T}\frac{\mathrm{D}\tilde{u}_i}{\mathrm{D}t} + \tilde{u}_i\frac{\mathrm{D}\tilde{T}}{\mathrm{D}t} \quad (26)$$

and formulate the terms on the right-hand side using the transport equations (23) and (24) as

$$\frac{\partial\tilde{u}_i\tilde{T}}{\partial t} + \frac{\partial}{\partial x_j}\left(\langle u_j\rangle^f\tilde{u}_i\tilde{T} + \tilde{T}\tilde{u}_i\tilde{u}_j - \alpha_f\tilde{u}_i\frac{\partial\tilde{T}}{\partial x_j}\right) = -\tilde{T}\tilde{u}_j\frac{\partial\langle u_i\rangle^f}{\partial x_j} - \tilde{u}_i\tilde{u}_j\frac{\partial\langle T\rangle^f}{\partial x_j} + \tilde{T}\left(-\frac{1}{\rho_f}\frac{\partial\tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i}\right)\right) - \alpha_f\frac{\partial\tilde{u}_i}{\partial x_j}\frac{\partial\tilde{T}}{\partial x_j} + \tilde{u}_i\frac{\partial}{\partial x_j}\langle\tilde{u}_j\tilde{T}\rangle + \tilde{T}\left(\frac{\nu_f}{K}\varepsilon\langle u_i\rangle^f + b\varepsilon^2(\langle u_k\rangle^f\langle u_k\rangle^f)^{1/2}\langle u_i\rangle^f\right) + \tilde{u}_i\frac{a_s h_f}{\varepsilon\rho_f c_{p_f}}(\langle T\rangle^f - \langle T\rangle^s) \quad (27)$$

where the deviation continuity equation (22) has been exploited. Then, carrying out the volume averaging treatment under the no-slip condition $\tilde{u}_i = -\langle u_i \rangle^f$ over the interface, we can derive the following transport equation for the dispersion heat flux after some manipulations:

$$\begin{aligned}
&\frac{\mathrm{D}\langle \tilde{u}_i \tilde{T} \rangle^f}{\mathrm{D}t} && \text{(convection)}\\
&+\frac{\partial}{\partial x_j}\left(\langle \tilde{T}\tilde{u}_i\tilde{u}_j \rangle^f - \alpha_f \left\langle \tilde{u}_i \frac{\partial \tilde{T}}{\partial x_j} \right\rangle^f \right) && \text{(diffusion)}\\
&= -\left(\langle \tilde{T}\tilde{u}_j \rangle^f \frac{\partial \langle u_i \rangle^f}{\partial x_j} + \langle \tilde{u}_i\tilde{u}_j \rangle^f \frac{\partial \langle T \rangle^f}{\partial x_j} \right) && \text{(production)}\\
&- \left\langle \alpha_f \frac{\partial \tilde{T}}{\partial x_j}\frac{\partial \tilde{u}_i}{\partial x_j} \right\rangle^f && \text{(dissipation)}\\
&+ \left\langle \tilde{T}\left(-\frac{1}{\rho_f}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right) \right\rangle^f . && \text{(redistribution)} \qquad (28)
\end{aligned}$$

The convection and diffusion terms on the left-hand side of (28) represent the spatial transport of the dispersion heat flux. As the divergence theorem indicates, these terms can influence the overall aspect of the thermal dispersion only through the events occurring on the boundaries. It is the first term on the right-hand side that is responsible for generating the dispersion heat flux by the gradients of the volume-averaged temperature and velocity, and thus, the term may be called the *production* term. The analogy between the dispersion heat flux and the turbulent wall heat flux indicates that the second and third terms on the right-hand side correspond to the *dissipation* and *redistribution* terms, respectively. These two terms almost balance with the production term. Thus, for the first approximation, we may neglect the spatial transport terms and obtain the following algebraic equation:

$$\begin{aligned}
&-\left(\langle \tilde{T}\tilde{u}_j \rangle^f \frac{\partial \langle u_i \rangle^f}{\partial x_j} + \langle \tilde{u}_i\tilde{u}_j \rangle^f \frac{\partial \langle T \rangle^f}{\partial x_j} \right) - \left\langle \alpha_f \frac{\partial \tilde{T}}{\partial x_j}\frac{\partial \tilde{u}_i}{\partial x_j} \right\rangle^f \\
&\qquad + \left\langle \tilde{T}\left(-\frac{1}{\rho_f}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right) \right\rangle^f = 0. \qquad (29)
\end{aligned}$$

4. Closure problem

Both dissipation and redistribution terms need some mathematical modelling to close the transport equation. According to a practice used in turbulence, a common way to model the redistribution term is to introduce the turbulent–turbulent interaction term (i.e. slow term) and turbulent–mean gradient interaction term (i.e. rapid term). However, it can easily be shown that the redistribution term must vanish for the tube flow problem, namely, the Taylor diffusion problem. This indicates that the term is negligible for most homogeneous macroscopic flows in porous media. Thus, one possible way to describe its overall mechanism is to retain only the rapid term

$$\left\langle \tilde{T}\left(-\frac{1}{\rho_f}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\nu_f \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right) \right\rangle^f = C_r \langle \tilde{u}_j \tilde{T} \rangle^f \frac{\partial \langle u_i \rangle^f}{\partial x_j}. \qquad (30)$$

If a transport equation is available for the dissipation rate $\langle \alpha_f (\partial \tilde{T}/\partial x_j)/(\partial \tilde{u}_i/\partial x_j)\rangle^f$, the set of macroscopic equations could be closed, since (29) along with (30) provides a complete set of algebraic equations for $\langle \tilde{u}_i \tilde{T}\rangle^f$. In this study, however, we do not try to obtain such a transport equation for the dissipation rate (as in the study of turbulence); instead, we seek an expression for the dissipation rate, which describes its fundamental mechanism. Upon noting that the dissipation rate increases with both the intensity of the dispersion heat flux $\langle \tilde{u}_k \tilde{T}\rangle^f$ and of $\langle \tilde{u}_i \tilde{u}_j\rangle^f$, we propose a very simple model, with its fundamental mechanism as follows:

$$\left\langle \alpha_f \frac{\partial \tilde{T}}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_j} \right\rangle^f = \beta_{jk} \langle \tilde{u}_i \tilde{u}_j\rangle^f \langle \tilde{u}_k \tilde{T}\rangle^f, \tag{31}$$

where β_{jk} is a symmetric tensor since the medium under consideration is a homogenous structure. Substituting (30) and (31) into (29) yields

$$-(1-C_r)\langle \tilde{T}\tilde{u}_j\rangle^f \frac{\partial \langle u_i\rangle^f}{\partial x_j} - \langle \tilde{u}_i \tilde{u}_j\rangle^f \left(\frac{\partial \langle T\rangle^f}{\partial x_j} + \beta_{jk} \langle \tilde{u}_k \tilde{T}\rangle^f \right) = 0. \tag{32}$$

When the flow is homogeneous, which is usually the case for flow in porous media, $\partial \langle u_i\rangle^f/\partial x_j$ may be neglected. Thus, dropping $(1-C_r)\partial \langle u_i\rangle^f/\partial x_j$, we obtain the effective thermal conductivity model as

$$\langle \tilde{u}_k \tilde{T}\rangle^f = -\beta_{jk}^{-1} \frac{\partial \langle T\rangle^f}{\partial x_j} \tag{33}$$

where $\beta_{ik}\beta_{jk}^{-1} = \delta_{ij}$. The foregoing expression reveals an obvious relationship between the dispersion thermal diffusivity tensor $(\alpha_{dis})_{ij}$ and the symmetric tensor β_{ij} as

$$(\alpha_{dis})_{ij} = \beta_{ij}^{-1}. \tag{34}$$

In this way, we can extract the gradient diffusion hypothesis commonly used for the thermal dispersion flux from its fundamental transport equation based on the Navier–Stokes and energy equations.

We note that the off-diagonal elements of the symmetric tensor β_{ij} are zero for isotropic media, and that β_{ij} is invariant with respect to the origin of the coordinate system. Considering these requirements and also the empirical fact implied by Fried & Combarnous (1971) that the axial dispersion element exceeds the transverse element roughly by a factor of 20, we propose one of the simplest tensor forms, as follows:

$$\beta_{ij} = \frac{1}{\alpha_{ax}} \frac{\langle u_i\rangle^f \langle u_j\rangle^f}{|\langle \vec{u}\rangle^f|^2} + \frac{C_{tr}}{\alpha_{ax}} \left(\delta_{ij} - \frac{\langle u_i\rangle^f \langle u_j\rangle^f}{|\langle \vec{u}\rangle^f|^2} \right) \tag{35}$$

where $C_{tr} \equiv \alpha_{ax}/\alpha_{tr} \sim 20$ is the ratio of the longitudinal dispersion coefficient to the transverse dispersion coefficient and $|\langle \vec{u}\rangle^f| = \sqrt{\langle u_k\rangle^f \langle u_k\rangle^f}$ is the magnitude of the intrinsic velocity vector (invariant in the transformation).

5. Determination of the coefficient α_{ax}

The coefficient α_{ax} may be determined from experiments, as a function of thermal diffusivity, local intrinsic velocity and morphological parameters. Such experimental investigations are needed for a variety of porous media. Nonetheless, it would be worthwhile to estimate it roughly from analytical consideration of a simple pressure-driven flow in a collection of circular tubes, as shown in figure 2, which corresponds

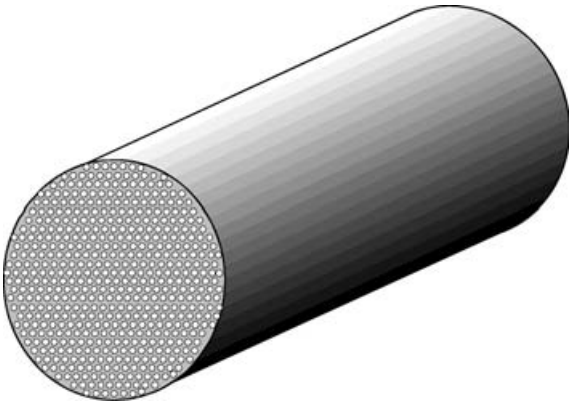

FIGURE 2. Flow through a bundle of circular tubes.

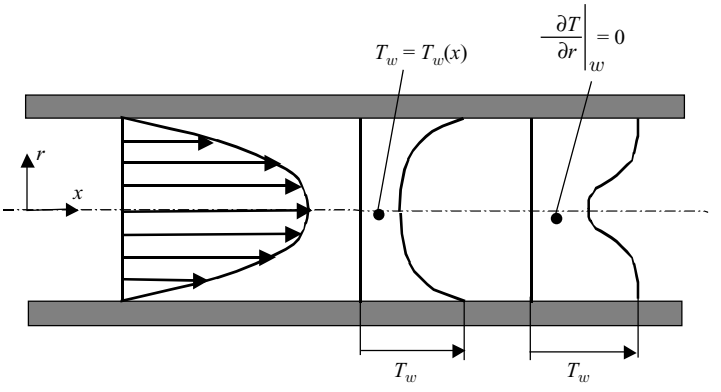

FIGURE 3. Velocity and temperature profiles in a tube.

to the Taylor dispersion model. Subsequently, we shall seek a possible extension to the case of heat and fluid flow in a packed bed.

Substituting (35) into (31), we obtain

$$\left\langle \alpha_f \frac{\partial \tilde{T}}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_j} \right\rangle^f = \beta_{jk} \langle \tilde{u}_i \tilde{u}_j \rangle^f \langle \tilde{u}_k \tilde{T} \rangle^f$$

$$= \frac{1}{\alpha_{ax}} \langle \tilde{u}_i \tilde{u} \rangle^f \langle \tilde{u} \tilde{T} \rangle^f + \frac{C_{tr}}{\alpha_{ax}} (\langle \tilde{u}_i \tilde{v} \rangle^f \langle \tilde{v} \tilde{T} \rangle^f + \langle \tilde{u}_i \tilde{w} \rangle^f \langle \tilde{w} \tilde{T} \rangle^f). \quad (36)$$

5.1. *Laminar flow case* (*Low Péclet number regime*)

We assume a macroscopically unidirectional flow through a bundle of tubes (i.e. Hagen–Poiseuille flow), as illustrated in figure 2, in which the both velocity and temperature profiles are fully–developed, as illustrated in figure 3, such that

$$u_i = (\langle u \rangle^f f(\eta),\ 0,\ 0) \quad (37)$$

and

$$T - T_w = (\langle T \rangle^f - T_w) g(\eta) \quad (38)$$

where $\eta = r/R$ is the dimensionless radial coordinate. Since the microscopic flow (in a tube) is unidirectional, its deviations are also unidirectional and thus the

thermal dispersion from a macroscopic viewpoint is expected to be purely axial. Upon substituting these expressions in (36), we find

$$\alpha_{ax} = \frac{\langle \tilde{u}^2 \rangle^f \langle \tilde{u}\tilde{T} \rangle^f}{\left\langle \alpha_f \dfrac{\partial \tilde{T}}{\partial r} \dfrac{\partial \tilde{u}}{\partial r} \right\rangle^f} = \frac{\langle (f-1)^2 \rangle^f \langle (f-1)(g-1) \rangle^f}{\left\langle \dfrac{\mathrm{d}f}{\mathrm{d}\eta} \dfrac{\mathrm{d}g}{\mathrm{d}\eta} \right\rangle^f} \alpha_f \left(\frac{\langle u \rangle^f R}{\alpha_f} \right)^2. \tag{39}$$

As we specify the profile functions $f(\eta)$ and $g(\eta)$, we can easily calculate the proportionality constant associated with α_{ax}.

Let us assume the following functions describing the fully developed velocity and temperature profiles:

$$f(\eta) = 2(1-\eta^2) \tag{40}$$

and

$$g(\eta) = (3/4)(3-4\eta^2+\eta^4) \tag{41}$$

which is the profile we would obtain for constant wall heat flux. Noting that

$$\langle \phi \rangle^f = 2\int_0^1 \eta \phi(\eta)\,\mathrm{d}\eta \tag{42}$$

such that $\langle f \rangle^f = \langle g \rangle^f = 1$, and substituting these profile functions into (39), we readily obtain

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} = \frac{1}{64}\left(\frac{\langle u \rangle^f R}{\alpha_f} \right)^2. \tag{43}$$

This expression should hold for most cases of thermal non-equilibrium, since the temperature profile given by (41) allows net heat transfer through a solid–fluid interface. The resulting proportionality constant 1/64 is very close to 1/60 obtained by Golfier *et al.* (2002) using their method of volume averaging.

Taylor (1953) considered the rate of spreading of the thick disk of mass content using a transformed axial coordinate, and obtained an expression for the axial dispersion coefficient with functional form identical to (43) but with its proportional constant being 1/48, which is somewhat larger than the foregoing value 1/64. This is due to the difference in the boundary condition at the tube wall. Taylor assumed that the species does not penetrate through the wall, which corresponds to the case of an adiabatic wall as illustrated in figure 3. One possible functional form would be

$$g(\eta) = 3(1-\eta^2)^2 \tag{44}$$

such that it satisfies $\mathrm{d}g/\mathrm{d}\eta|_{\eta=1} = 0$ and $\langle g \rangle^f = 1$ in addition to the symmetric condition. We substitute the temperature profile function given by (44) along with the fully developed velocity profile function given by (40) into (39) and then find an expression identical to that of Taylor:

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} = \frac{1}{48}\left(\frac{\langle u \rangle^f R}{\alpha_f} \right)^2. \tag{45}$$

This expression should hold for most cases of thermal equilibrium, since the temperature profile prohibits any heat from transferring through the interface between the solid and fluid.

5.2. *Turbulent flow case* (*High-Péclet-number regime*)

De Lemos & Pedras (2001) showed using their double-decomposition theory that either a time–space or space–time order of application of averaging operators

is immaterial for deriving the macroscopic momentum and energy equations for turbulent flow in porous media. However, the two different orders of applying operators lead to two distinct definitions of macroscopic turbulence kinetic energy, namely, the volume average of the Reynolds-averaged turbulence kinetic energy and the time-averaged kinetic energy of the volume-averaged fluctuating velocity components. Guo *et al.* (2003) applied three different models based on the former definition, namely, those of Nakayama & Kuwahara (1999), de Lemos & Pedras (2001) and Takeda (1994), to the gas flow in a circular packed column of spheres and validated them against one another and against experimental data in the literature. They reported that these models predict widely different turbulent eddy diffusivity, with the model by Nakayama & Kuwahara being the best in predicting a reasonable eddy diffusivity. Therefore, we start with the Reynolds-averaged version of the governing equations (such as derived by Nakayama & Kuwahara 1999) so as to form the transport equation for the thermal dispersion heat flux vector associated with deviations of the microscopic Reynolds-averaged velocity and temperature. On the other hand, the turbulent microscopic dispersion associated with both time and spatial deviations (which is most likely to be negligible compared to the aforementioned dispersion) could be modelled together with turbulent mixing (Rocamora & de Lemos 2000) and thus requires no transport equation.

It is straightforward to start with the Reynolds-averaged version of the governing equations (see Nakayama & Kuwahara 1999 for details) and follow the decomposition and volume averaging procedure as illustrated for the case of laminar flow. The resulting expression is

$$\alpha_{ax} = \frac{\langle\tilde{u}^2\rangle^f\langle\tilde{u}\tilde{T}\rangle^f}{\left\langle\left(\alpha_f + \frac{\nu_t}{\sigma_T}\right)\frac{\partial\tilde{T}}{\partial r}\frac{\partial\tilde{u}}{\partial r}\right\rangle^f} \simeq \frac{\langle\tilde{u}^2\rangle^f\langle\tilde{u}\tilde{T}\rangle^f}{\left\langle\frac{\nu_t}{\sigma_T}\frac{\partial\tilde{T}}{\partial r}\frac{\partial\tilde{u}}{\partial r}\right\rangle^f} = \frac{\langle\tilde{u}^2\rangle^f\langle\tilde{u}\tilde{T}\rangle^f}{\left\langle\frac{q_t}{\rho_f c_{pf}}\frac{\partial u}{\partial r}\right\rangle^f} \tag{46}$$

where u and T are the Reynolds-averaged velocity and temperature, respectively. Furthermore, q_t, ν_T and σ_T are the turbulent heat flux, turbulent kinematic viscosity and turbulent Prandtl number, respectively. The wall laws may be used:

$$u = u_\tau\left(\frac{1}{\kappa}\ln n^+ + B\right) \tag{47}$$

and

$$T - T_w = \frac{q_w\sigma_T}{u_\tau\rho_f c_{pf}}\left(\frac{1}{\kappa}\ln n^+ + A\right) \tag{48}$$

where u_τ and q_t are the friction velocity and wall heat flux, respectively, and $n^+ = u_\tau n/\nu_f$ is the dimensionless distance measured from the wall ($n = R - r$). κ is the von-Kármán constant while both B and A are empirical constants. It is easy to find

$$\tilde{u} = \frac{u_\tau}{\kappa}\left(\ln\zeta + \frac{3}{2}\right) \tag{49}$$

and

$$\tilde{T} = \frac{q_w\sigma_T}{u_\tau\rho_f c_{pf}\kappa}\left(\ln\zeta + \frac{3}{2}\right) \tag{50}$$

noting that

$$\langle\phi\rangle^f = 2\int_0^1 \eta\phi(\zeta)\,\mathrm{d}\eta = 2\left(\int_0^1 \phi(\zeta)\,\mathrm{d}\zeta - \int_0^1 \zeta\phi(\zeta)\,\mathrm{d}\zeta\right) \tag{51}$$

where

$$\zeta = n/R = 1-\eta. \tag{52}$$

Using profile functions (49) and (50), we have

$$\langle\tilde{u}^2\rangle^f\langle\tilde{u}\tilde{T}\rangle^f = \frac{u_\tau^2\sigma_T q_w}{\kappa^4\rho_f c_{pf}}\left(\left\langle\left(\ln\zeta+\frac{3}{2}\right)^2\right\rangle^f\right)^2 = \left(\frac{5}{4}\right)^2\frac{u_\tau^2\sigma_T q_w}{\kappa^4\rho_f c_{pf}} \tag{53}$$

and

$$\left\langle\frac{q_t}{\rho_f c_{pf}}\frac{\partial u}{\partial r}\right\rangle^f \simeq \left(\frac{q_w}{\rho_f c_{pf}}\right)\left(\frac{u_\tau}{\kappa R\zeta_{ref}}\right) = \frac{q_w u_\tau}{\rho_f c_{pf}\kappa R\exp\left(-\frac{1}{2}(3-\sqrt{5})\right)} \tag{54}$$

where

$$\left(\ln\zeta_{ref}+\frac{3}{2}\right)^2 = \left\langle\left(\ln\zeta+\frac{3}{2}\right)^2\right\rangle^f = \frac{5}{4}. \tag{55}$$

Since the wall law fails towards the laminar sublayer, we have exploited the constant stress and heat flux approximation valid for the equilibrium turbulent boundary layer, namely, $q_t \simeq q_w$ and $\mathrm{d}u/\mathrm{d}n \simeq u_\tau/\kappa n$. Substituting (53) and (54) into (46), we have

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} \simeq \left(\frac{5}{4}\right)^2 \mathrm{e}^{-(3-\sqrt{5})/2}\,\frac{\sigma_T}{\kappa^3}\left(\frac{u_\tau R}{\alpha_f}\right) \simeq 14\left(\frac{u_\tau R}{\alpha_f}\right) \tag{56}$$

where κ and σ_T are set to 0.41 and 0.9, respectively, according to Launder & Spalding (1974). Expression (56) is very close to Taylor's (1954) one:

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} \simeq 10.06\left(\frac{u_\tau R}{\alpha_f}\right). \tag{57}$$

Upon substituting the Blasius friction law:

$$\lambda_f \equiv \left(-\frac{\mathrm{d}\langle p\rangle^f}{\mathrm{d}x}\right)\Big/\left(\frac{\rho_f(\langle u\rangle^f)^2}{4R}\right) = \frac{8\tau_w}{\rho_f(\langle u\rangle^f)^2} = 0.3164\left(\frac{\langle u\rangle^f 2R}{\nu_f}\right)^{-1/4} \tag{58}$$

into (56), we obtain an approximate expression for the axial dispersion coefficient as follows:

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} \simeq 14\left(\frac{u_\tau R}{\alpha_f}\right) = 14\sqrt{\frac{\lambda_f}{8}}\left(\frac{\langle u\rangle^f R}{\alpha_f}\right) \simeq 2.55\left(\frac{\langle u\rangle^f R}{\alpha_f}\right)^{7/8} Pr^{1/8}. \tag{59}$$

The two distinct expressions (43) and (59) obtained for the low- and high-Péclet-number limiting cases are presented in figure 4 for the case of $Pr = 1$, in which the two lines intersect at $\langle u\rangle^f R/\alpha_f = 93Pr^{1/9}$. Since the high-Péclet-number expression depends only weakly on Pr, the transition Péclet number may be roughly estimated as $\langle u\rangle^f R/\alpha_f = 100$ for most fluids, irrespective of the value of Pr.

6. Extension to the case of dispersion in a packed bed

We have determined the thermal dispersion coefficients for heat transfer in a bundle of tubes, which provided an excellent test for the closure problem associated with the present transport equation based on the volume averaging theory. The idea of using

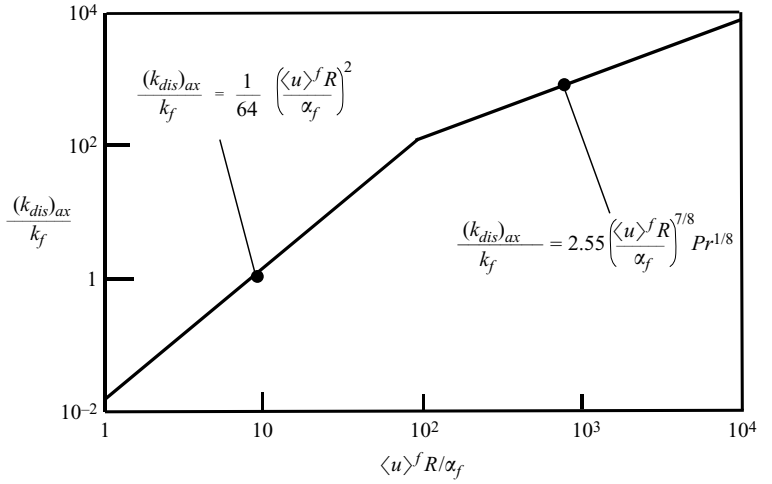

FIGURE 4. Axial thermal dispersion coefficient for low- and high-Péclet-number cases at $Pr = 1$.

tubes to obtain insight into complex transport processes in real porous media has been explored in the past by a number of researchers such as Taylor (1953) and Aris (1956). Although the limits associated with such a simple system as a bundle of tubes must certainly be born in mind, a possible extension of the foregoing results to a packed bed may still be worthwhile. The empirical evidence for porous media, namely, the axial dispersion element predominating over the transverse element, supports such an extension based on a bundle of tubes in which the latter element virtually vanishes.

Thus, we may generalize the foregoing results to the case of dispersion in a packed bed. Nakayama, Kuwahara & Motoyama (2004*b*) introduced an analogy between the tube flow and the flow through a packed bed, to translate the results obtained for the tube flows to the cases of packed beds. They rewrite Ergun's (1952) empirical formula for a unidirectional flow through a packed bed:

$$-\frac{\mathrm{d}\langle p\rangle^f}{\mathrm{d}x} = \frac{150\,(1-\varepsilon)^2}{\varepsilon^2 d_p^2}\mu_f\langle u\rangle^f + 1.75\frac{1-\varepsilon}{\varepsilon d_p}\rho_f(\langle u\rangle^f)^2 \tag{60}$$

to conform with the Poiseuille formula as

$$\lambda_{eq} \equiv \left(-\frac{\mathrm{d}\langle p\rangle^f}{\mathrm{d}x}\right)\Big/\left(\frac{\rho_f(\langle u\rangle^f)^2}{2d_{eq}}\right) = \frac{64}{Re_{d_{eq}}} + 1.62 \tag{61}$$

where

$$Re_{d_{eq}} \equiv \frac{\langle u\rangle^f d_{eq}}{\nu_f} = \sqrt{\frac{32}{150}}\frac{\varepsilon}{1-\varepsilon}\frac{\langle u\rangle^f d_p}{\nu_f} \tag{62}$$

is the Reynolds number based on the equivalent tube diameter which is related to the particle diameter d_p as

$$d_{eq} = 2R = \sqrt{\frac{32}{150}}\frac{\varepsilon}{1-\varepsilon}d_p. \tag{63}$$

From a comparison of the numerical results obtained for arrays of square cylinders (Nakayama, Kuwahara & Hayashi 2004*a*) with the foregoing friction coefficient formula they concluded that Ergun's formula, when based on the equivalent tube diameter, is a universal law that can be used for most two- and three-dimensional

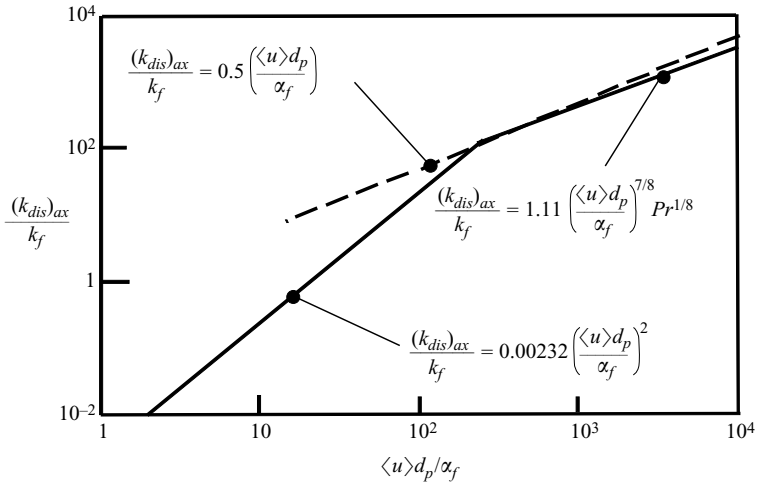

FIGURE 5. Comparison of the present formula with the empirical formula for packed beds for $Pr = 1$.

periodic structures in a wide porosity range. We shall exploit this equivalent tube diameter concept as

$$\frac{\langle u\rangle^f R}{\alpha_f} = \sqrt{\frac{4}{75}}\frac{\varepsilon}{1-\varepsilon}\frac{\langle u\rangle^f d_p}{\alpha_f} = \sqrt{\frac{4}{75}}\frac{1}{1-\varepsilon}\frac{\langle u\rangle d_p}{\alpha_f} \cong 0.385\frac{\langle u\rangle d_p}{\alpha_f} \tag{64}$$

where the porosity for a packed bed is assumed to be $\varepsilon = 0.4$ and $\langle u\rangle d_p/\nu_f$, commonly used for a packed bed, is the particle Reynolds number based on the particle diameter d_p and Drcian velocity $\langle u\rangle = \varepsilon\langle u\rangle^f$. Upon substituting the foregoing relationship into (43) and (59), we obtain the following expressions for the packed beds:

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} = 0.00232\left(\frac{\langle u\rangle d_p}{\alpha_f}\right)^2 \quad \text{(for the low-Péclet-number regime)}, \tag{65}$$

$$\frac{\alpha_{ax}}{\alpha_f} = \frac{(k_{dis})_{ax}}{k_f} \simeq 1.11\left(\frac{\langle u\rangle d_p}{\alpha_f}\right)^{7/8} Pr^{1/8} \quad \text{(for the high-Péclet-number regime)}. \tag{66}$$

These expressions for the packed beds are presented in figure 5 along with the empirical formula proposed by Yagi *et al.* (1960) for a packed bed in a high-Péclet number range, namely,

$$\frac{(k_{dis})_{ax}}{k_f} = 0.5\left(\frac{\langle u\rangle d_p}{\alpha_f}\right) \quad \text{(empirical (Yagi } et\ al.\ 1960)). \tag{67}$$

Our high-Péclet-number expression (66) for the axial dispersion coefficient, despite the difference in the Reynolds number dependence, closely follows the empirical formula established by Yagi *et al.* This substantiates the validity of the present extension based on the equivalent tube diameter.

In this analysis, a simple tube flow model has been adopted, and then the results have been translated to packed beds using the concept of equivalent tube diameter. The results are valid for packed beds with porosity around 0.4. But it should be noted that the present correlations may fail to hold for other cases such as highly porous media or more complex structural geometries.

7. Conclusions

In this study, the gradient diffusion hypothesis for thermal dispersion heat flux has been examined in terms of its transport equation derived from the Navier–Stokes and energy equations. It has been shown that the differential transport equation can be reduced to an algebraic transport equation if we drop the spatial transport terms. The gradient diffusion expression usually adopted for the thermal dispersion heat flux can be generated naturally from this algebraic transport equation. The Taylor diffusion problem, namely, a macroscopically unidirectional flow through a tube, has been considered to determine the unknown model constants. It has been found that Taylor's expression for the axial dispersion is obtainable if we assume adiabatic tube walls. Both laminar and turbulent flow cases are investigated to obtain two distinct limiting expressions for low- and high-Péclet-number regimes. The results obtained for tube flow are translated to the case of flow in a packed bed to obtain the corresponding expressions for the axial dispersion coefficient in a packed bed. The resulting expression for the high-Péclet-number case agrees well with the empirical formula established by Yagi *et al.*

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