Theoretical formalism and closure for turbulence modelling in a random anisotropic medium

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Résumé - En industrie chimique, de nombreuses applications reposent sur le passage d'un écoulement turbulent à travers des assemblages non-structurés. L'exemple d'un tube chauffé rempli de catalyseurs sphériques peut être pris comme un prototype pour comprendre les transferts thermiques dans de tels systèmes. D'un point de vue statistique ce système peut être modélisé par un milieu poreux avec une porosité constante au coeur mais présentant une forte variation près des parois. Nous proposons ici une extension du modèle de turbulence macroscopique $\langle k \rangle - \langle \epsilon \rangle$ pour prendre en compte les phénomènes induits par le gradient de porosité radial sur l'écoulement turbulent, la dispersion et le transport thermique ainsi que les caractéristiques du volume représentatif approprié pour ce type de milieu.

Nomenclature

C_p	specific heat of fluid at constant pressure, J/Kg/K
d	REV thickness in the radial direction, m
L	REV size in the axial direction, m
l_0	pore length scale, m
L_0	macroscopic characteristic length scale, m
l_{REV}	REV characteristic length scale, m
k	turbulent kinetic energy, m^2/s^2
K	macroscopic kinetic energy, m^2/s^2
n_i	normal vertor component in the i direction
p	pressure, Pa
r_{tube}	tube raidus, m
S	solid surface, m^2
T	temperature of the homogeneous medium, K
T_f	fluid temperature, K
T_s	solid temperature, K
u_i	velocity component in the i direction, m/s
V	representative elementary volume, m^3
Greek Symbols	
$\delta.$	spatial deviation
ϵ	dissipation rate, m^2/s^3
ϕ	porosity
φ	general physical quantity
λ_f	fluid conductivity, W/m/K
λ_s	solid conductivity, W/m/K
λ_{eff}	fluid effective conductivity, W/m/K
ν	fluid kinematic viscosity, m^2/s
ν_T	effective kinematic viscosity in homogeneous isotropic medium, m^2/s
ν_{TOT}	effective kinematic viscosity in homogeneous anisotropic medium, m^2/s
ρ_f	fluid density, Kg/m^3
σ_t	turbulent Prandtl number
Operators	
$\langle . \rangle$	volume averaging operator
$\bar{.}$	time averaging operator

1. Introduction

In chemical engineering, numerous process consist in turbulent flowing through structured or unstructured bunch of particles. For instance, tubular reactors based on a cylindrical heated tube randomly filled with catalyst particles in which flows a high Reynolds fluid (1000 to 10000 Re) is a typical industrial process. The understanding of physical mechanisms occurring in such systems is essential for tubular reactors design and process optimisation. The main purpose of this study is to better assess the near wall heat transfer. Recent developments in macroscopic turbulence modeling in porous medium based namely on volume averaging methods and up scaling approaches have significantly improved the understanding of heat[2, 1] and mass[3, 5] transfer in structured and unstructured[16] isotropic medium. Nevertheless, physical mechanisms occurring in the near wall area remain not well understood yet. It is needless to say that near wall area is particularly interesting as it involves complex physical mechanisms such as boundary layer effects, interaction between porous medium/boundary layer or high porosity gradient which impact widely mass and heat transfer over this area. The main scope of this paper is to capture the effect of the porosity gradient on turbulent flow. Hence, it is suggested here, a theoretical formalism which intends to extend the existing high Reynolds turbulence models for anisotropic porous medium.

2. Macroscopic Turbulence model in isotropic porous medium

2.1. Volume averaging concept [14, 15]

As far as turbulent flows are involved, the time averaging operator is applied to instantaneous flow governing equations in order to separate the evolution of mean flow quantities from fluctuation quantities (RANS formulation).

$$\varphi = \bar{\varphi} + \varphi' \tag{1}$$

where φ and $\bar{\varphi} = \frac{1}{\Delta t}\int_t^{t+\Delta t} \varphi dt$ are the instantaneous and time averaged quantities and φ' the time fluctuation around the mean quantity. Using the same reasoning, one can apply the volume averaging procedure to obtain macroscopic flow governing equations through a porous medium. The quantity is averaged over a volume which is large enough to be statistically meaningful to represent the medium and at the same time small enough compared to the characteristic length scale L_0 of spatial variations of macroscopic quantities.

$$l_0^3 \ll V \ll L_0^3 \tag{2}$$

where l_0 is the characteristic length scale of microscopic quantities. Such a volume V is called *Representative Elementary Volume* (REV). It is worthwhile noting that variations of volume averaged quantities over REVs are smooth and represent the mean behaviour in the homogeneous medium.

$$\langle\varphi\rangle^v = \frac{1}{V}\int_V \varphi \, dV \tag{3}$$

where $\langle\varphi\rangle^v$ is the volume averaged quantity. Hence,

$$\varphi = \langle\varphi\rangle^i + \delta\varphi \tag{4}$$

where $\langle\varphi\rangle^i$ is the intrinsic averaged value of the quantity for the fluid phase inside the representative elementary volume V and $\delta\varphi$ its spatial deviation. The volume average and the intrinsic volume average for the fluid phase are both related by

$$\langle\varphi\rangle^v = \phi\langle\varphi\rangle^i \tag{5}$$

where ϕ is the porosity of the medium, ($\phi = V_F/V$, with V_F the volume of fluid within the REV).

It is also worth nothing that the volume average of derivatives is not equal to the derivatives of volume average.

$$\langle\nabla\varphi\rangle^v = \nabla\langle\varphi\rangle^v + \frac{1}{V}\int_{A_i} \mathbf{n}\varphi \, dS \tag{6}$$

$$\langle \nabla.\varphi \rangle^v = \nabla.\langle \varphi \rangle^v + \frac{1}{V}\int_{A_i} \mathbf{n}.\varphi \, dS \tag{7}$$

To describe a turbulent flow through a porous (homogeneous) medium, one can apply both time and volume averaging operators to an instantaneous flow quantity φ. Furthermore, it can be showed that the application's order of averaging operators is immaterial for a rigid medium,

$$\langle \bar{\varphi} \rangle = \overline{\langle \varphi \rangle} \tag{8}$$

Applying the double decomposition to a general flow quantity, one can obtain

$$\varphi = \langle \bar{\varphi} \rangle + \langle \varphi' \rangle + \delta\bar{\varphi} + \delta\varphi' \tag{9}$$

and the scale separation's assumption between microscopic and macroscopic quantities leads to

$$\langle \delta\varphi \rangle = \bar{\varphi}' = 0 \tag{10}$$

2.2. Macroscopic turbulence modeling in isotropic porous medium ($\phi_0 = cte$)

Applying the double averaging operator to the momentum and energy equation one can obtain,

$$\phi_0[\frac{\partial}{\partial t}\langle \bar{u}_i \rangle^i + \frac{\partial}{\partial x_j}(\langle \bar{u}_j \rangle^i \langle \bar{u}_i \rangle^i)] = -\phi_0 \frac{\partial}{\partial x_i}\frac{\langle \bar{p} \rangle^i}{\rho_f} + \phi_0 \nu \frac{\partial^2}{\partial x_j^2}\langle \bar{u}_i \rangle^i - \phi_0 \frac{\partial}{\partial x_j}[\underbrace{\langle \overline{\delta u_j \delta u_i} \rangle^i}_{dispersive\ flux\ density} + \underbrace{\langle \overline{u_j' u_i'} \rangle^i}_{turbulent\ flux\ density}] \underbrace{- \frac{1}{V\rho_f}\int_{A_i} n_i \bar{p} dS + \frac{\nu}{V}\int_{A_i} n_j \frac{\partial \overline{u_i}}{\partial x_j} dS}_{drag\ force} \tag{11}$$

where the drag force at the solid surface is usually substituted by the Darcy-Forchheimer law[4, 6, 7, 8] and,

$$\begin{aligned}
&[(\rho C_p)_f \phi_0 + (\rho C_p)_f (1-\phi_0)]\frac{\partial}{\partial t}\langle \bar{T} \rangle^i + (\rho C_p)_f \frac{\partial}{\partial x_i}(\phi_0 \langle u_i \rangle^i \langle \bar{T} \rangle^i) = \\
&\frac{\partial}{\partial x_i}\Big[(\lambda_f \phi_0 + \lambda_s(1-\phi_0))\frac{\partial}{\partial x_i}\langle \bar{T} \rangle^i + \underbrace{\frac{1}{V}\int n_i(\lambda_f \bar{T}_f - \lambda_s \bar{T}_s) ds}_{tortuosity} \\
&- \phi_0 (\rho C_p)_f [\underbrace{\langle \overline{\delta u_i \delta T} \rangle^i}_{heat\ dispersion} + \underbrace{\langle \overline{u_i' T'} \rangle^i}_{turbulent\ heat\ flux\ density}]\Big]
\end{aligned} \tag{12}$$

where the tortuosity is usually negligible.

Although Nakayama et al.[8] proposed to apply the volume averaging operator to the microscopic TKE, Teruel et al. [9, 10, 11] have recently highlighted the dispersive kinetic energy (DKE) leading hence to a new definition of the macroscopic turbulent kinetic energy,

$$\langle K \rangle^i = \langle k \rangle^i_{RANS} + \frac{1}{2}\langle \delta\bar{u}\delta\bar{u} \rangle^i \tag{13}$$

While Pinson et al.[13] writing a transport equation for the dispersive part highlighted energy transfer between TKE and DKE, Mathey[16] following Teruel et al. suggestions has successfully assessed mass and heat transfer in the isotropic part of an unstructured porous medium expanding the usual Boussinesq approximation as

$$\phi_0[\langle\overline{\delta u_j \delta u_i}\rangle^i + \langle\overline{u'_j u'_i}\rangle^i] = -\langle\nu_T\rangle^i[\frac{\partial\phi_0\langle\overline{u_i}\rangle^i}{\partial x_j} + \frac{\partial\phi_0\langle\overline{u_j}\rangle^i}{\partial x_i}] + \phi_0\frac{2\langle K\rangle^i}{3}\delta_{ij} \tag{14}$$

with

$$\rho_f\langle\nu_T\rangle^i = \rho_f C_\mu \frac{\langle K\rangle^i\langle K\rangle^i}{\langle\epsilon\rangle^i} \tag{15}$$

and,

$$-(\rho C_p)_f[\langle\overline{\delta u_i \delta T}\rangle^i + \langle\overline{u'_i T'}\rangle^i] = \lambda_{eff}\frac{\partial}{\partial x_i}\langle\bar{T}\rangle \tag{16}$$

with

$$\lambda_{eff} = (\rho C_p)_f\frac{\langle\nu_T\rangle^i}{\sigma_t} = (\rho C_p)_f\frac{C_\mu\langle K\rangle^i\langle K\rangle^i}{\sigma_t\langle\epsilon\rangle^i} \tag{17}$$

3. Macroscopic Turbulence model in anisotropic porous medium

The scope of this section is to expand the results obtained above to a porous medium presenting an anisotropy in the radial direction such as in the vicinity of wall within tubular reactors. When one considers the porosity gradient, new terms appear in Eq.11,

$$\nu\langle\bar{u}_i\rangle^i\frac{\partial^2}{\partial x_j^2}\phi + [2\nu\frac{\partial}{\partial x_j}\langle\bar{u}_i\rangle^i - \langle\overline{u'_j u'_i}\rangle^i - \langle\overline{\delta u_j \delta u_i}\rangle^i - \langle\bar{u}_i\rangle^i\langle\bar{u}_j\rangle^i]\frac{\partial}{\partial x_j}\phi \tag{18}$$

and in Eq.12,

$$(\lambda_f - \lambda_s)\langle\bar{T}_i\rangle^i\frac{\partial^2}{\partial x_j^2}\phi + [2(\lambda_f - \lambda_s)\frac{\partial}{\partial x_j}\langle\bar{T}\rangle^i - \langle\overline{T' u'_j}\rangle^i - \langle\overline{\delta T \delta u_j}\rangle^i - \langle\bar{u}_j\rangle^i\langle\bar{T}\rangle^i]\frac{\partial}{\partial x_j}\phi \tag{19}$$

which require modeling efforts. Neglecting the second order term, Eq.18 can be summed up as $\psi\nabla_j\phi$ with ψ the quantity carried away by $\nabla_j\phi$. As the physical mechanism induced by the porosity gradient is a spatial transfer, one can write it as a flux divergence,

$$\psi_0\frac{\partial\phi}{\partial x_i}\mid_{x_0} \quad \approxeq \quad \frac{\partial\left[\psi\frac{\partial\phi}{\partial x_i}\mid_{x_0} d\right]}{\partial x_i}\mid_{x_0} \tag{20}$$

where d is the thickness of the REV. Thus, adding Eq.18 up to Eq.11, the effective viscosity is extended as,

$$\begin{aligned}\langle\nu_{TOT}\rangle_M^i = &\underbrace{\nu\left[1 + \frac{2\nabla_j\phi}{\phi}C_{diff}^{(1)}d\right]}_{Molecular\quad diffusion} + \underbrace{\langle\nu_T\rangle^i\left[1 + \frac{\nabla_j\phi}{\phi}C_T^{(1)}d\right]}_{Turbulent\quad diffusion} \\ &-\underbrace{\frac{\nabla_j\phi}{\phi}r_{tube}C_{cv}^{(1)}\langle\bar{u}_j\rangle^i d}_{Convection}\end{aligned} \tag{21}$$

where r_{tube} is the tube radius and $C_{diff}^{(1)}$, $C_T^{(1)}$ and $C_{cv}^{(1)}$ are model constants. Then, the effective conductivity is written as,

$$\lambda_{eff} = (\rho C_p)_f\frac{\langle\nu_{TOT}\rangle_M^i}{\sigma_t} \tag{22}$$

To be valid this approach set constraints on the REV. Indeed, the REV's size in the porosity gradient direction d has to be smaller than an interval Δx_j around a point x_0 wherein the porosity function $\phi(x_j)$ can be substituted by its linear approximation $\phi(x_j) \approxeq \phi(x_0) + \nabla_j \phi \mid_{x_0} \Delta x_j$.

However, approaching walls the porosity gradient becomes steep and the associated interval $\Delta x_j \mid_{nearwall}$ shrinks to pore scales, making the volume statistically inappropriate to represent the medium. One can think to extend the other directions of the REV such as it covers statistically enough configurations to be representative of the considered medium. That is to say when d shrinks, L is increased in size as to keep the volume V large enough so that the characteristic length scale $l_{REV} = V^{1/3}$ remains larger than the pore scale l_0 (Figure 1). Hence, the constraints induced on the REV can be written as,

$$d \leq Min(\Delta x_j) \quad and \quad l_{REV} >> l_0 \tag{23}$$

For usual flow conditions ($Re \simeq 8000$), mass (Figure 2a and Figure 2b) and heat (Figure 3a and Figure 3b) REV-averaged fluxes are estimated from microscopic simulations. It is worthwhile nothing that fluxes carried out by porosity gradient would seem to damp mass and heat transfer in the radial direction.

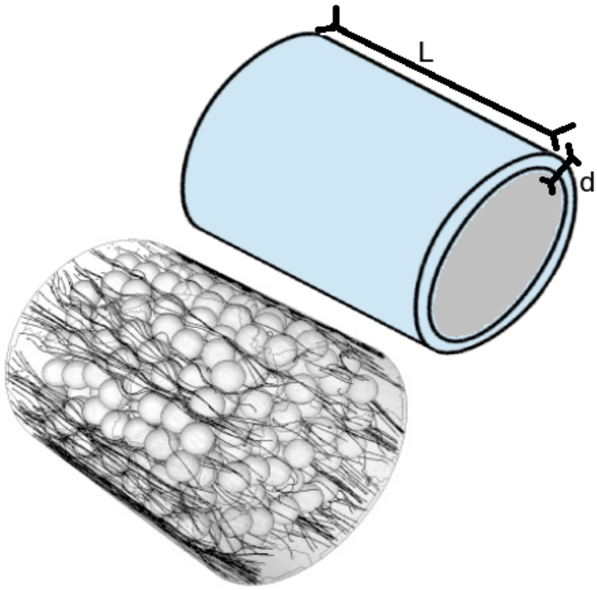

Figure 1 : *Statistically meaningful REV for tubular reactor.*

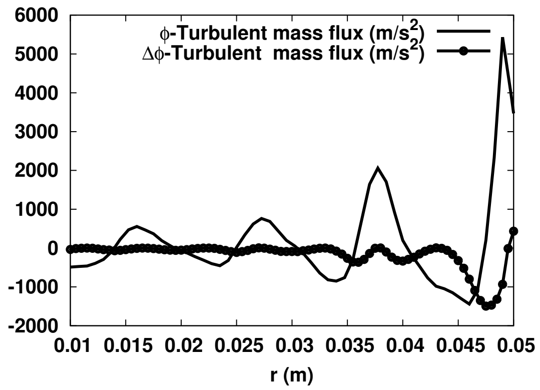

Figure 2a : *Radial profile of turbulent mass transfer at* $Re \simeq 8000$.

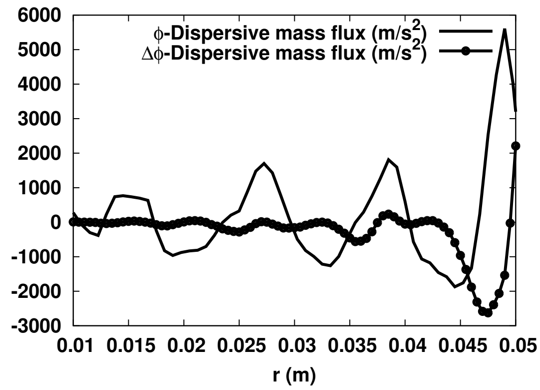

Figure 2b : *Radial profile of dispersive mass transfer at* $Re \simeq 8000$.

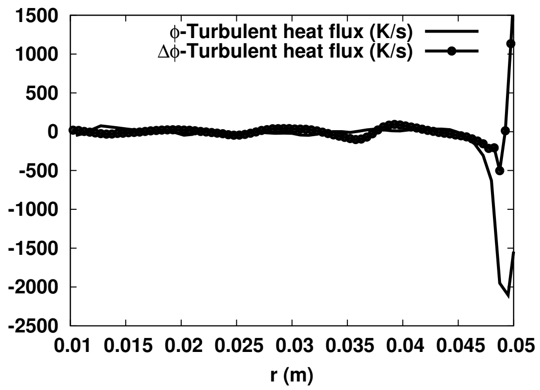

Figure 3a : *Radial profile of turbulent heat transfer at* $Re \simeq 8000$.

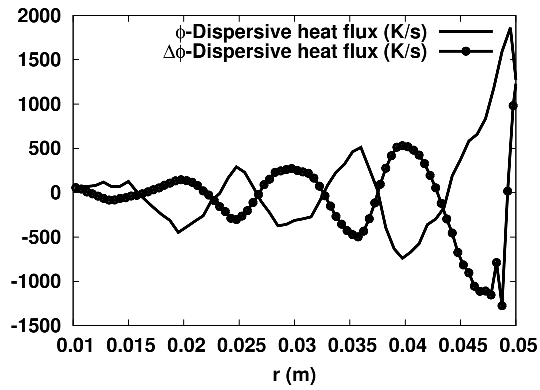

Figure 3b : *Radial profile of dispersive heat transfer at* $Re \simeq 8000$.

4. Conclusion

A new formalism is presented to include porosity gradient effect on turbulence modeling in porous medium which is numerically assessed to be responsible for the damping of radial mass and heat transfer especially in the vicinity of walls. Works are in progress to tune model coefficients and to assess the radial anisotropy effect on the macroscopic kinetic energy $\langle K \rangle$ and the macroscopic dissipation rate $\langle \epsilon \rangle$. Furthermore, all these developments will be used to assess accurately the near wall heat transfer in realistic packed beds.

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