



## Numerical investigation on the thermal non-equilibrium in low-velocity reacting flow within porous media



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### ABSTRACT

This paper addresses the thermal non-equilibrium problem for a low-velocity reacting flow within isotropic porous media. The method of volume-averaging is employed to derive the macroscopic thermal transport equation for the fluid phase inside the porous medium including a heat source due to a homogenous chemical reaction, which is then closed by representing the temperature deviation through a constitutive equation. Theoretical treatment indicates that the contribution of the non-equilibrium due to reaction heat to the macroscopic heat transfer comes up in terms of an additional energy source rather than affecting thermal transport properties. Through dimensional analysis, this term can be interpreted as a convective transport of the reaction heat. Numerical computations are conducted by solving the closure problems at the pore scale for the fluid phase in a spatially periodic representative elementary volume (REV). Simulation results show that the convective coefficient related with the reaction heat is dependent on the Thiele modulus number, and the arrangement of cylinders. For the inline case, when the Péclet number is less than 10, a part of reaction heat will feed back to the upstream due to local conductivity, for Péclet number greater than 10 this part of energy will be transmitted to the downstream. For the staggered case, the same conclusion holds for smaller Péclet number, while the non-equilibrium will gradually decay to zero as the Péclet number increases. In addition, the other effective coefficients, such as effective conductivity, surface convective heat transfer coefficient are calculated with and without inertia.

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### 1. Introduction

According to the difference of the superficial averaging temperatures between fluid and solid phases, models for heat transfer occurring in porous media can be categorized into local thermal equilibrium and non-equilibrium models. Strictly speaking, when the difference among the local temperature of the phases is comparable in magnitude to the temperature difference across the length scale the local thermal non-equilibrium occurs [1]. For a heat exchanger, since there is no heat generation, so generally, it is treated as the local thermal equilibrium in the case that far from the system boundaries. However, as stated in Kaviany's monograph [2], when a significant heat generation is of existence, the local thermal equilibrium will break down, and double separated phase averaging equations for solid and fluid will be necessary for the description of the heat transfer process. Moreover, Quintard

and Whitaker [3] provided a number of physical situations that the local thermal equilibrium could be failed in their researches.

The thermal non-equilibrium can be characterized by the heat transfer between the solid and fluid phases, which is closely related to the Darcy velocity and geometrical characteristic of the matrix as well as thermal physical properties, such as specific heat capacity, thermal conductivity, and so on. For the creeping flow or low Reynolds number laminar flow, the thermal conduction is the most important factor affecting heat transfer, so the total thermal conductivity comprising of thermal dispersion conductivity and stagnant effective conductivity is sufficient to describe the process. With the Darcy velocity increasing, the convection will gradually replace thermal conduction, and become a dominant element. Simultaneously, the thermal dispersion due to hydraulic mixing overcomes molecular diffusion and plays a significant role on the enhancement of heat transfer.

Dispersion phenomena including two aspects of heat and mass have been extensively studied both theoretically and experimentally. Hsu and Cheng [4] proposed that axial thermal dispersion conductivity is linearly proportional to the Péclet number in the range of high Reynolds numbers, while it has a quadratic

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## Nomenclature

$a_{fs}$	specific surface area of the interface of fluid-to-solid within a REV, $m^{-1}$
$A_{fs}$	the interface of fluid-to-solid
$\mathbf{b}$	closure parameter, m
$\mathbf{c}$	closure parameter, m
$c_p$	specific heat capacity, J/(kg K)
$\mathbf{f}$	closure parameter, m
$h$	sensible enthalpy, J/kg
$h_{fs}$	convective heat transfer coefficient on the interface, W/ $m^2$ K
$H$	the characteristic length of unit cell, m
$k$	turbulent kinetic energy, $m^2/s^2$
$k_f$	thermal conductivity, W/(m K)
$k_h$	homogeneous reaction rate constant, $s^{-1}$
$\mathbf{K}_d$	thermal dispersion tensor, W/(m K)
$\mathbf{K}_{eff}$	effective thermal conductivity tensor, W/(m K)
$l$	length scale related with an averaging volume, m
$L$	macroscopic length scale related with the considered system, m
$\mathbf{n}$	unit normal vector
$Nu$	Nusselt number, $Nu = a_{fs}h_{fs}H^2/k_f$
$Pe$	Péclet number defined by $Pe = u_p H/\alpha_f$
$Re$	Reynolds number defined by $Re = u_p H/\nu$
$t$	time, s
$t^*$	time scale associated with temperature deviation, $\tilde{T}_f$ , s
$T$	temperature, K
$\mathbf{u}$	velocity vector, m/s
$u_p$	characteristic velocity, m/s
$V$	volume, $m^3$
$\mathbf{x}$	position vector within the REV, m
$\Delta\mathbf{x}$	periodic length vector of REV, m
$Y_i$	mass fraction of the $i$ th species

## Greek symbols

$\alpha$	thermal diffusivity, $m^2/s$
$\varepsilon$	porosity or turbulent kinetic energy dissipation
$\phi$	any effective coefficient involved in this paper
$\varphi$	closure parameter
$\eta$	relative error between with and without inertia
$\mu_t$	turbulent eddy viscosity, $N s/m^2$
$\nu$	kinetic viscosity of fluid phase, $m^2/s$
$\rho$	density of fluid phase, $kg/m^3$
$\tau$	Thiele modulus, $\tau^2 = k_h H^2/\alpha_f$
$\psi$	any physical variable associated with fluid phase
$\Omega$	the inner region of the REV

## Subscript

$f$	fluid phase
$fe$	the enter or exit of the REV
$M$	macroscopic scale
$r$	term related with chemical reaction heat
$s$	solid phase
$w$	interface of fluid and solid phases

## Superscripts

$*$	dimensionless form of a variable
$T$	transposition of a matrix

## Others

$\sim$	spatial deviation of a variable
$\langle \rangle$	volume averaging
$\langle \rangle^r$	$\gamma$ -phase volume averaging
$\Delta h_c$	chemical reaction heat, J/kg

dependence on the velocity for low Reynolds numbers. Kuwahara and Nakayama [5] considered the effect of porosity and proposed a set of empirical correlations, which also have the same dependence on the Péclet number as Hsu and Cheng, though some distinction existing in the expressions for the longitudinal dispersion within different range of the Péclet number. However, for the transversal dispersion, if the Péclet number based on the diameter is less than 10, Nakayama's result also shows a quadratic dependence on the Péclet number. Pedras and de Lemos [6] investigated thermal dispersion and showed that thermal dispersion is a function of solid-to-fluid conductivity ratio. For the longitudinal dispersion, it decreases with the ratio increasing in an exponential relationship,  $Pe^m$ , where  $Pe$  is based on the length of unit cell,  $m$  equals 1.65; while for the transversal dispersion,  $m$  takes values of 0.94 and 0.88 for  $k_s/k_f = 10$  and 2, respectively. Moyne et al. [7] employed a new concept, namely *average temperature of the medium* by replacing the condition that the mean temperature deviations is equal to zero, getting a one-equation model for describing the thermal dispersion process inside porous media. In addition, Nakayama et al. [8] developed an equation for thermal dispersion flux with the volume-averaging method which provides rigid constraints that the gradient diffusion hypothesis can be satisfied. A series of empirical correlations were established by Delgado [9] based on more than five hundred experimental data and through an exhaustive compilation and a critical analysis of the mass dispersion data, which are measured in packed beds of mono-sized particles and constant voidage, with both air and water as the fluid phase. For the case of liquid flows, the author used a division into five and four dispersion regimes to obtain

expressions for longitudinal and transversal dispersion, respectively. In the case of gas, due to its Schmidt number is close to unity, the author quoted the results of previous studies. It is worth to note that the tortuosity was treated as an important parameter affecting mass dispersion in his study. Furthermore, Wood [10] paid a particular attention on the influence of inertial contribution on the mass dispersion at moderated Reynolds numbers. Their results show that the inertial effect on the longitudinal dispersion coefficient is relatively small, but for the transversal dispersion coefficient, the inertial effect can increase it up to 40 times as big as that predicted by Stokes flow. More elaborate reviews on dispersion can be found in Refs. [9,11].

On convective heat transfer in porous media, many studies have been conducted in the last five decades. Most of the obtained empirical correlations are in the form of  $Re^m Pr^n$ , for instance the result by Wakao and Kaguei [12]. Kuwahara et al. [13] resorted to the numerical method to determine the convective heat transfer coefficient of porous media with periodic structure. In their correlation, the porosity was introduced as an independent parameter. Later on, in Saito and de Lemos's [14] research, the influence of porosity on the convective heat transfer was confirmed again. Izadpanah et al. [15] experimentally investigated the convective heat transfer in a cylindrical porous medium with the conclusion that the natural convection could be neglected with respect to the forced convection and it is related to the flow velocity rather than to the thermal flux. Alshare et al. [16] considered the influence of flow angles on convective heat transfer for the square rod arrangement. Contrast to the in-line configuration, it is more closely dependent on the Reynolds number for the case of staggered

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