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# Direct numerical simulation of non-isothermal flow through dense bidisperse random arrays of spheres

H. Tavassoli, E.A.J.F. Peters*, J.A.M. Kuipers

*Multiphase Reactors Group, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, MB Eindhoven 5600, The Netherlands*

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ABSTRACT

Extensive direct numerical simulations were performed to obtain the heat transfer coefficients (HTC) of bidisperse random arrays of spheres. We have calculated the HTC for a range of compositions and solids volume fractions for mixtures of spheres with a size ratio of 1:2. The Reynolds numbers are in the range of 30–100. It was found that the correlation of the monodisperse HTC can estimate the average HTC of bidisperse systems well if the Reynolds and Nusselt numbers are based on the Sauter mean diameter. We report the difference between the HTC for each particle type and the average HTC of the bed in the bidisperse system as function of solids volume fraction, Sauter mean diameter of the mixture, Reynolds number and investigate the heterogeneity of the individual particle HTCs.



## 1. Introduction

Packed and fluidized beds have received considerable interest for many engineering applications due to their abilities to provide high rates of momentum and heat transfer. Key parameters that determine the momentum and heat transfer characteristics inside packed and fluidized beds are the drag and heat transfer coefficients (HTC). In order to predict these coefficients experimental correlations have been widely used. For example, the available experimental and computational data of pressure drop and HTC (for randomly packed beds of spheres) agree reasonably well with the predictions of traditional empirical correlations such as Ergun [6] and Wakao and Kaguei [16].

However, many correlations are obtained for mono-disperse random arrays of spheres. In reality, the particles can have a significant size distribution. For example, the particles can grow as consequence of physical (coating) and chemical (polymerization) processes in fluidized suspensions. Therefore, these momentum and heat transfer correlations may result in a significant error if the average deviation of the particle size from the mean value is not negligible.

An accepted approach, in the case of non-uniform spheres, is to use an average particle size. For example, Balakrishnan and Pei [1] suggest a simple arithmetic average value whilean area-volume average for the particle diameter of the bed is suggested by de Souza-Santos [4]. Despite such modifications, the numerical simulations show significant deviation with experimental results [2,11]. Therefore, no concrete approaches have been proposed to characterize the heat transfer in polydisperse systems.

To date, most of the correlations are based on experimental data. It is a difficult task to measure the effect of polydispersity on the drag force or heat transfer experimentally, in particular when the effect on individual particle types must be considered.

Accurate prediction of fluid-solid flows needs improved thermal and hydrodynamic models, which require better understanding of the effect of polydispersity. Unlike multiphase experimental techniques, direct numerical simulation (DNS) can provide detailed information at the small scale in multiphase systems. One of the biggest advantages of DNS is that the operating conditions can be perfectly controlled, which is often not the case in experiments. Based on accurate numerical data from lattice-Boltzmann simulations Hill et al. [9] and Van der Hoef et al. [10] proposed new drag force relations. Van der Hoef et al. [10] and Beetstra et al. [3] conducted extensive DNS to characterize the drag force in mono- and bidisperse arrays of spheres. They proposed a correlation for the drag force applicable to both mono- and polydisperse systems, based on the Carman-Kozeny equations. Recently, the mono- and polydisperse systems were studied by other researchers as well (such as [14,17]) and new correlations were proposed.

DNS has been extended to heat transfer problems [5,12,15] and the HTC was estimated for the fixed random arrays of monodispersed spherical particles. These results show significant deviations between numerical HTC and prediction of empirical correlations even in beds with mono-disperse spherical particles.

* Corresponding author.
*E-mail address:* E.A.J.F.Peters@tue.nl (E. Peters).

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To the authors knowledge, no numerical study has been performed to investigate heat transfer in polydisperse systems of spherical particles. In this paper, a first step is made towards assessment of the effect of polydispersity on the heat transfer in packed and fluidized beds. The focus of our study is on binary systems, although it can be extended readily to polydisperse systems.

The numerical approach that we employ here is similar to the approach used by Tavassoli et al. [12] to measure the HTC in monodisperse systems. DNS approach has been employed to simulate bidisperse systems. In the DNS approach, the fluid and solid phases are treated by considering the Navier-Stokes equations and the Newtonian equations of motion (for particles that move), respectively. The mutual interactions between the phases are obtained by enforcing the appropriate boundary conditions at the surface of the particle (e.g. no-slip and Dirichlet boundary condition for momentum and heat transfer, respectively) and no empirical correlations are required. Consequently the DNS approach can improve our insight regarding the effect of non-ideality on the hydrodynamic and thermal behaviors of the multiphase system. In this study, we employ the immersed boundary (IB) method to simulate non-isothermal flows through a fixed bed packed with random bidisperse spherical particles. The physical model is constructed by distribution of 54 non-overlapping spherical particles in a cubic domain using a standard Monte Carlo procedure for hard spheres . A cold fluid flows through the hot particles in the bed and interchanges the heat and momentum with particles. From the detailed flow and thermal fields, information on the average and distribution of the heat transfer coefficient of the system can be obtained.

The paper is organized as follows. First, the governing equations and numerical solution method are discussed. Next, the HTCs of fixed random arrays of bidisperse systems are determined based on the Sauter mean diameter and then compared with well-known correlations. Then the HTC of each type of particle is characterized as well. The conclusions are provided in the last section.

## 2. Physical model and numerical method

### 2.1. Physical model

The physical domain is a 3-dimensional duct that consists of an inlet, packed and outlet section, as shown in Fig. 1a. A total of 54 non-overlapping spherical particles, with $N_S$ spheres of diameter $D_S$ and $N_L = 54 - N_S$ spheres of diameter $D_L$, are distributed randomly in the packed section by means of a Metropolis Monte Carlo procedure (subscripts $L$ and $S$ denote large and small particles, respectively). The diameter ratio that was considered is $D_S : D_L = 1 : 2$. By changing the relative amount of small and large particles, i.e. $N_S : N_L$, the influence of the composition on the heat transfer is investigated. The packed section has dimensions $L \times L \times L$ and the sizes of inlet and outlet sections are the same and set to $D_L \times L \times L$ for all simulations in this study. The desired size $L$ for a given solids volume fraction $\phi$ can be determined from $\phi = \frac{\pi}{6}\left(N_S D_S^3 + N_L D_L^3\right)/L^3$.

The cold fluid flows enters with a temperature $T_0$ and flows through the duct in the (streamwise) $x$-direction. In spanwise ($y$ and $z$) directions periodic boundary conditions are imposed to avoid wall effects. All spheres are maintained at a constant temperature $T_s$ and exchange energy with the flowing fluid. Therefore only the packed section is active in heat transfer. The fluid physical properties are assumed to be independent of temperature.

The following Navier-Stokes and thermal energy equations were solved for an unsteady incompressible fluid flow with constant physical properties and negligible viscous heating effects:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u} = -\rho^{-1}\vec{\nabla}p + \nu\nabla^2\vec{u} + \vec{f}_{\mathrm{IB}} \tag{1}$$

$$\vec{\nabla}\cdot\vec{u} = 0 \tag{2}$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T = \nu\,\mathrm{Pr}^{-1}\nabla^2 T + Q_{\mathrm{IB}}, \tag{3}$$

where $\rho$, $\nu$, $\vec{u}$, $T$ and $p$ are the density, kinematic viscosity, velocity field, temperature and pressure of the fluid, respectively. The Prandtl number, Pr, is taken to be 1 and the fluid kinematic viscosity and fluid density are set to $10^{-5}$ m$^2$/s and 1 kg/m$^3$ in all simulations. The source terms $\vec{f}_{\mathrm{IB}}$ and $Q_{\mathrm{IB}}$ represent the hydrodynamic and thermal fluid-solid interactions, respectively.

The boundary conditions for this simulation were set as follows:

- At the inlet ($x = 0$), uniform axial velocity $U$ and temperature $T_0$ of the fluid are imposed:

$$u_y = u_z = 0,\ u_x = U, \text{ and } T = T_0. \tag{4}$$

- At the outlet ($x = X$), the boundary conditions are:

$$\frac{\partial \vec{u}}{\partial x} = 0,\ \frac{\partial T}{\partial x} = 0. \tag{5}$$

- On the periodic boundaries:

$$\begin{aligned} &\vec{u}(x,0,z) = \vec{u}(x,Y,z),\ T(x,0,z) = T(x,Y,z)\\ &\vec{u}(x,y,0) = \vec{u}(x,y,Z),\ T(x,y,0) = T(x,y,Z) \end{aligned} \tag{6}$$

  where Y and Z are the size of domain in y and z directions, respectively.
- At the particle surface, Dirichlet conditions were used for the velocity (no-slip) and temperature,

$$\vec{u} = 0,\ T = T_s. \tag{7}$$

To minimize the influence of the inlet and outlet boundary conditions the inlet and outlet sections as shown in Fig. 1a were added. By varying their size and monitoring the influence on the results it was found that the results were invariant for inlet and outlet regions of length $D_L$ or larger.

### 2.2. Numerical method

The simulation of this system had been performed by using the immersed boundary method (IBM) extended to handling heat transfer. This method is explained in detail in Tavassoli et al. [12]. Therefore, we describe it only briefly in this section. In IBM, the fluid occupies the whole domain, even inside the particles, and is modeled on the fixed Eulerian grid. The momentum and energy equations are discretized and solved by the finite difference method on this staggered Eulerian grid. A fractional-step method is used to integrate the equations in time. A particle is represented by Lagrangian points uniformly distributed over the outer boundary of the particle (Fig. 1b).

The mutual hydrodynamic and thermal interactions between the fluid and the particle are modeled by introducing the volume forcing and volumetric heat source terms in momentum and energy equations, respectively. These terms are calculated such that the desired boundary conditions are satisfied on the immersed boundary (i.e. no-slip velocity and Dirichlet boundary conditions). In each time step, the immersed boundary source terms are calculated at the Lagrangian points and then they are distributed to the neighbor Eulerian grid nodes by means of regularized delta-functions. These

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