Moving from momentum transfer to heat transfer – A comparative study of an advanced Graetz-Nusselt problem using immersed boundary methods

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Highlights

- Fully resolved simulations of heat transfer problems in tubular fluid-particle systems.
- Handles mixed boundary conditions, i.e. isothermal and isoflux, consistently.
- Investigation of the influence of particle sizes and passive particles.
- Comparison between two classes of immersed boundary method, i.e. CFM and DFM.

Abstract

In this paper two immersed boundary methods (IBM), specifically a continuous forcing method (CFM) and a discrete forcing method (DFM), are applied to perform direct numerical simulations (DNSs) of heat transfer problems in tubular fluid-particle systems. Both IBM models are built on the well-developed models utilized in momentum transfer studies, and have the capability to handle mixed boundary conditions at the particle surface as encountered in industrial applications with both active and passive particles.

Following a thorough verification of both models for the classical Graetz-Nusselt problem, we subsequently apply them to study a much more advanced Graetz-Nusselt problem of more practical importance with a dense stationary array consisting of hundreds of particles randomly positioned inside a tube with adiabatic wall. The influence of particle sizes and fractional amount of passive particles is analyzed at varying Reynolds numbers, and the simulation results are compared between the two IBM models, finding good agreement. Our results thus qualify the two employed IBM modules for more complex applications.
1. Introduction

Tubular fluid-particle flows are frequently encountered in a wide range of processes in chemical, petrochemical and energy industries. A typical example is the catalytic packed bed reactor, where the reaction takes place on the surface of catalysts and most of the time heat is liberated. The random packing of the particles leads to a strongly irregular flow pattern inside the bed, and the heat transport process introduces additional complexities to such highly heterogeneous systems. In case a reaction is mildly exothermic or temperature insensitive, adiabatic operation is applied such that the bed is surrounded by an insulating jacket. In the past decades, numerous empirical correlations for fluid-particle heat transfer have been proposed building on experimental studies. After Ranz and Marshall (1952) had published the first correlation for the single particle system, Gupta and Thodos (1963), Daizo and Motoyuki (1967), Nelson and Galloway (1975), Gunn (1978), Hughmark (1980), Kumar and Fan (1994) and many other researchers contributed to the development of heat transfer correlations for both packed and fluidized systems consisting of multiple particles. These correlations are very helpful to quantify the average heat transfer rate for the design purpose of the process equipment, however, they are often limited to specific operating conditions. Moreover, detailed information regarding local transport phenomena cannot be provided. Under these circumstances, three dimensional transient computer simulations are useful because of their capability to produce quantitative information instead of an average value.

With the fast development of computational methods and power in recent years, DNS has demonstrated its ability to resolve all details at the smallest relevant length scales to gain fundamental insight into fluid-solid interactions and quantitatively derive microscale transport coefficients for application in coarser scale models.

In this context the overset grid method proposed by Chesshire and Henshaw (1990) is a crucial technique, which can incorporate the fluid-solid interaction accurately, however problems arise when the body-conforming grids partially overlap. Hu et al. (2001) proposed the arbitrary Lagrangian-Eulerian technique whose advantage is also the accurate incorporation of the fluid-solid interaction, but an expensive remeshing operation is unavoidable. Another DNS technique is the Lattice-Boltzmann method (Ladd, 1994a,b; van der Hoef et al., 2005), which however has several disadvantages including a mandatory calibration of particle radii and complications to implement general transport equations.

In comparison to all these DNS techniques, the immersed boundary method (IBM) has recently received a lot of attention due to its clear merits of easy grid generation and efficient CPU and memory utilization. Fadlun et al. (2000), Kim et al. (2001), Peskin (2002), Iaccarino and Verzicco (2003), Uhlmann (2005), Mittal and Iaccarino (2005), Xu and Wang (2006), Wang et al. (2008), Kajishima and Takeuchi (2011), Xu et al. (2013), Spandan et al. (2017) and many other researchers have applied it in various studies including complex geometries, moving particles and deformable immersed objects. One more significant advantage of IBM, which will be utilized in this paper, is that an additional equation for thermal energy transport or for scalar transport can be added with relative ease, using the same methodology following the fluid flow equations.

The IBM was introduced by Peskin (1977) for the simulation of blood flow around the flexible leaflet of the human heart. In this technique a Cartesian grid is used to solve the fluid field and Lagrangian marker points are used for the representation of the immersed object. In case of moving or deformable particles, the Lagrangian marker points are associated with the motion of the object surface. A forcing term is introduced in the momentum conservation equation to represent the interaction between the
immersed object and the fluid, whose magnitude is taken such that the no-slip boundary condition are fulfilled in an interpolated manner. This singular force is distributed over the Eulerian cells surrounding each Lagrangian point through a regularized Dirac delta function. In this technique the fluid-solid coupling is treated explicitly at the level of the undiscretized equation, hence it is classified as the continuous forcing method (CFM). Goldstein et al. (1993), Saiki and Biringen (1996), Uhlmann (2005), Takeuchi et al. (2010), Spandan et al. (2017) and many other researchers contributed to the further development of this technique. A different class of the IBM technique is the discrete forcing method (DFM), which was first proposed by Mohd-Yusof (1997) and later extended by Fadlun et al. (2000), Udaykumar et al. (2001), Tseng and Ferziger (2003), Mittal et al. (2008), Deen et al. (2012). In DFM Lagrangian marker points are not used any more, and the interaction between the immersed boundary and the fluid is accounted for at the level of the discretized equations. In most cases, ghost cells (i.e.: cells inside the solid phase but required for the solution of the liquid phase equations) are defined and their virtual variable values are calculated by applying boundary conditions to extrapolate fluid variables near the boundary to the ghost cells. DFM treats the immersed boundary as a sharp interface and does not require the explicit addition of a discrete force in the governing equations, and hence the stability conditions are the same as that without the treatment of the immersed boundaries.

Contrary to the vast literature on the IBM techniques applied for the study of momentum transfer in fluid-solid systems, limited results have been reported for heat transfer processes in gas-solid flows. Feng and Michaelides (2009) studied a group of 56 settling particles with time dependent temperature in a 2D domain. The particles are represented and tracked by Lagrangian points, and an energy density function is used to represent the interaction between the fluid and solid phase. Deen et al. (2012) applied 3D DFM with a directional quadratic interpolation scheme to fluid flow and heat transfer problems in dense fluid-particle systems involving stationary particle arrays and fluidized particles. The boundary condition of a constant temperature at the particle surface is enforced implicitly at the level of the discrete fluid thermal energy equation. Tenneti et al. (2013) proposed a CFM for the heat transfer study in steady flow past random assemblies of stationary particles. The isothermal boundary condition is enforced at the particle surface, and a special periodic boundary condition is implemented in the flow direction to obtain a statistically homogeneous Nusselt number. Tavassoli et al. (2013) extended the Uhlmann method to study the interphase heat transport of stationary arrays which consist of 54 spheres with packing fraction varying from 0.1 to 0.5. A constant temperature is enforced at the sphere surface and a heat source term is added into the governing equation to account for the fluid-solid interaction. Xia et al. (2014) studied the fluid-solid heat transfer for a cluster consisting of 20 manually configured spheres. A ghost-cell based third-order IBM is introduced to enforce the isothermal boundary condition at the reactor wall and a conjugate heat transfer is considered at the particle surface for the computation of the temperature fields in both solid and fluid phases.

In this paper both of these two immersed boundary methods, CFM and DFM, are employed to perform simulations of fluid-particle systems inside a tube. The direct comparison of these two methods is of high interest to reveal their consistency. Building on the well-developed models for the momentum computation, both IBM models are extended to include thermal energy transport. The interaction between the tube and the fluid is treated exactly the same as the fluid-particle interactions. As a pronounced merit, both of our models have the capability to handle mixed boundary conditions at the immersed object surface. Taking this advantage, both isothermal and isoflux boundary conditions can be enforced consistently at the particle surface as well as the tube wall.

The organization of this paper is as follows. First, the descriptions of both IBM models are given, including the governing equations and the numerical solution methods (Section 2). The classical (and analytically solvable) Graetz-Nusselt problem is then simulated to serve as a detailed verification of the codes. After that a much more advanced and technically relevant Graetz-Nusselt problem is studied, namely by positioning a stationary dense particle array inside a tube with adiabatic wall. In both IBM methods the heat transfer process is analyzed and the results of the two IBM models are compared against each other, finding good agreement (Section 3). Finally, in Section 4, the conclusions are presented.

2. Model description

We first describe the governing equations that need to be solved in DNS. Subsequently, the numerical details as well as the fluid-solid coupling are introduced for both CFM and DFM models. For the models presented in this paper, the following main assumptions are applied:

1. The fluid phase is incompressible and Newtonian.
2. The solid phase consists of spherical particles. In case of active particles, a uniform temperature is enforced at the external surface.
3. Both fluid and solid phase have constant physical properties, and the thermal effect on the fluid density is not considered.

2.1. Governing equations

The transport phenomena in the fluid phase are governed by the conservation equations for mass, momentum and thermal energy, respectively defined as:

\[ \nabla \cdot \mathbf{u} = 0. \]  
\[ \frac{\partial \rho_f \mathbf{u}}{\partial t} + \nabla \cdot (\rho_f \mathbf{u} \mathbf{u}) = -\nabla p + \mu_f \nabla^2 \mathbf{u} + \rho_f \mathbf{g}. \]  
\[ \rho_f C_p \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{T} \mathbf{u}) = \lambda_f \nabla^2 T_f. \]

In above equations, \( \rho_f \) is the fluid density, \( \mu_f \) is the fluid viscosity, and \( C_p, T_f, \) and \( \lambda_f \) are the heat capacity and thermal conductivity of the fluid phase, respectively.

2.2. Numerical methods

In both CFM and DFM models, the above governing equations are solved by a finite difference scheme implemented for a staggered Cartesian grid, which possesses a uniform grid spacing in all three directions. To advance the velocity field, the pressure gradient is solved through a two-step projection method: an intermediate velocity field is first computed by using the pressure at the
2.2.1. CFM model

In the CFM model, the pressure is calculated at the center of the grid while the temperature field is located on the face of the vertical velocity. The momentum equation is discretized by applying the Adams-Bashforth scheme for the convective term and the Crank-Nicholson scheme for the diffusive term, as given by the following expression:

\[
\rho \mathbf{u}^{n+1} = \rho \mathbf{u}^{n} + \Delta t \left[ - \frac{\partial p}{\partial x} + \tau \mathbf{C}_m + \rho \gamma C_m^{-1} \frac{\partial }{\partial x} \left( \frac{D_m^x + D_m^y}{2} \right) + \rho \mathbf{g} \right].
\] (4)

In this equation, \( n \) is the time step index. Time marching is performed with a fractional step third order Runge-Kutta (RK3) scheme and \( \tau \), \( \gamma \), and \( \rho \) are the coefficients of the time advancement scheme and the same values as \( \text{Rai and Moin (1991)} \) have used. The convective and diffusive momentum fluxes \( \mathbf{C}_m \) and \( \mathbf{D}_m \) are calculated by spatial discretization of:

\[
\mathbf{C}_m = \rho \left( \nabla \cdot \mathbf{u} \right),
\] (5)

\[
\mathbf{D}_m = \mu \nabla^2 \mathbf{u}.
\] (6)

Both the convection and diffusion terms are spatially discretized by a standard second-order central differencing scheme. The implicit treatment of the diffusive term of \( \text{Eq. (4)} \) requires the solution of the inversion of large sparse matrices; they are reduced to three tridiagonal matrices by a factorization procedure with error \( O(\Delta t^2) \). The tridiagonal matrices can be solved by using FFT in the periodic boundaries to achieve fast computation. For more details of the fluid solver, we refer the readers to \( \text{Verzicco and Orlandi (1996)}, \text{van der Poel et al. (2015)}, \text{Zhu et al. (2018)} \). The thermal equation is discretized and solved exactly the same way as the momentum equation.

To keep track of the immersed objects inside the flow, a continuous forcing immersed boundary method has been implemented, based on the work of \( \text{Uhlmann (2005)} \). It should be noted that hydrodynamic radius calibration is not used in the current work. The idea is to add an Eulerian force term \( \mathbf{f} \) into the right hand side of \( \text{Eq. (4)} \). The fluid-solid interfaces have been discretized into a series of Lagrangian points. The Eulerian and Lagrangian forces are related to each other through a regularized delta function:

\[
\mathbf{f}(\mathbf{x}) = \int \mathbf{F}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}_f) \, d\mathbf{s},
\] (7)

where \( \mathbf{x} \) and \( \mathbf{x}_f \) are the position vectors of the Eulerian and Lagrangian points; \( \mathbf{F} \) the Eulerian force term; \( \delta \) the delta function; \( d\mathbf{s} \) the Lagrangian grid width, respectively. To enforce the non-slip boundary condition on the interface, a Lagrangian velocity field can be defined. We use the regularized delta function again:

\[
\int \mathbf{u}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}_f) \, d\mathbf{x} = \mathbf{V}_f(\mathbf{x}_f),
\] (8)

where \( \mathbf{V}_f \) is the Lagrangian velocity on the boundary. The Lagrangian force can be calculated when \( \mathbf{V}_f \) does not equal the prescribed velocity \( \mathbf{V}_p \) on the boundary:

\[
\mathbf{F} = \rho \left( \mathbf{V}_p - \mathbf{V}_f \right) \Delta t.
\] (9)

For the thermal boundary condition on the fluid-solid interface, an identical procedure can be adopted. Note that when dealing with the Neumann boundary condition, a probe which is perpendicular to the boundary and equals to one grid width is used to calculate the surface temperature based on the temperature gradient that is prescribed.

The regularized delta function used in the present study is defined as

\[
\delta(\mathbf{x} - \mathbf{x}_f) = \frac{1}{h^3} \phi \left( \frac{\mathbf{x} - \mathbf{x}_f}{h} \right).
\] (10)

where \( \phi \) in the present implementation is based on the four-point version of \( \text{Peskin (2002)} \) and \( h \) is the grid width which is the same in every direction.

\[
\phi(r) = \begin{cases} 
\frac{1}{h} \left( 3 - 2|r| + \sqrt{4 + 4|r| - 4r^2} \right), & |r| \leq 1, \\
\frac{1}{h} \left( 5 - 2|r| - \sqrt{7 + 12|r| - 4r^2} \right), & 1 \leq |r| \leq 2, \\
\frac{1}{h} (|r| - 2), & 2 \leq |r|. 
\end{cases}
\] (11)

2.2.2. DFM model

In the DFM model, the pressure and the temperature are both calculated at the center of the grid. The momentum equation is discretized by applying the Adams-Bashforth scheme for the convective term and the Euler backward scheme for the diffusive term, as given by the following expression:

\[
\rho \mathbf{u}^{n+1} = \rho \mathbf{u}^{n} + \Delta t \left[ - \frac{\partial p}{\partial x} + \frac{3}{2} \mathbf{C}_m^{-1} - \frac{1}{2} \mathbf{C}_m^{-1} + \frac{\partial }{\partial x} \left( \frac{D_m^x + D_m^y}{2} \right) + \rho \mathbf{g} \right].
\] (12)

As the same as the CFM model, \( n \) is the time step index, and the convective and diffusive momentum fluxes \( \mathbf{C}_m \) and \( \mathbf{D}_m \) are calculated by spatial discretization of Eqs. (5) and (6). However, in the DFM model, the convection term is spatially discretized by a second-order total variation diminishing scheme, whereas the diffusion term is computed with a standard second-order central differencing scheme. The thermal energy equation is temporally and spatially discretized in the same way as for the momentum equation.

The discretization of momentum and thermal energy equations leads to algebraic equations in the following generic form:

\[
a_c \phi_c + \sum_{i=1}^{6} a_{ic} \phi_{ic} = b_c,
\] (13)

where \( \phi \) is the fluid variable for which we want to find a solution, namely velocity and temperature fields for momentum and thermal energy equation, respectively. This equation provides the relationship between the fluid variable \( \phi_c \) at the central position and the variables at its six neighbors \( \phi_{ic} \). This results in a seven-diagonal sparse matrix, which is solved by a Block-Incomplete Cholesky Conjugate Gradient solver efficiently (Deen et al., 2012; Das et al., 2017b).

Since the surfaces of the immersed objects do not coincide with the mesh boundaries, a special treatment is required for the boundary condition enforcement at the fluid-solid interface. For this purpose, ghost points are applied, which locate inside the solid phase but possess at least one neighbor in the fluid phase. Every fluid point is checked whether any of its six surrounding neighbors represents a ghost point. If this is the case, the prescribed boundary condition has to be incorporated into the virtual ghost value, which is then used to update the coefficients in a sparse matrix and sequentially obtain a solution of the fluid phase governing equations. In our DFM model, a second order quadratic interpolation scheme is applied, which allows the enforcement of the Robin boundary condition at the exact particle surface. In this paper we briefly introduce the essential concepts, while the full methodology of this method can be found in our earlier publication (Lu et al., 2018a).
A generic variable $\phi$ in the vicinity of the immersed object surface can be approximated in terms of a second-order polynomial as follows:

$$\phi = \sum_{i=0}^{2} \sum_{j=0}^{2} \sum_{k=0}^{2} c_{ijk} x^i y^j z^k, \quad i + j + k \leq 2,$$

(14)

where $x, y$ and $z$ are relative coordinates with respect to the origin located at the boundary point. This equation is in fact the approximation of $\phi$ using the Taylor expansion near the boundary point:

$$\phi(x,y,z) = \phi_0 + \frac{\partial \phi_0}{\partial x} x + \frac{\partial \phi_0}{\partial y} y + \frac{\partial \phi_0}{\partial z} z + \frac{1}{2} \frac{\partial^2 \phi_0}{\partial x^2} x^2 + \frac{1}{2} \frac{\partial^2 \phi_0}{\partial y^2} y^2 + \frac{1}{2} \frac{\partial^2 \phi_0}{\partial z^2} z^2 + \cdots.$$  

(15)

Comparing above two equations, one can clearly see that all the information required for the Robin boundary condition

$$a \phi_0 + b \frac{\partial \phi_0}{\partial n} = f,$$

(16)

are stored in the first four coefficients, namely the surface value and its derivative in $x, y$ and $z$ direction respectively. The ten coefficients $c_{ijk}$ can be determined by ten data points, namely $\phi$ values at nine neighboring fluid points and one image point, which results in the equation written as:

$$\phi = Xc,$$

(17)

where $\phi$ and $c$ are the vectors for variables and coefficients respectively, and $X$ is the Vandermonde matrix consisting of the information regarding the relative coordinates. The coefficients $c_{ijk}$ are obtained by multiplication of the inverted Vandermonde matrix and the variable vector, which can be written as a linear combination of $\phi$ values. With that, the value at the image point can be first back-calculated, from which the ghost value can be finally obtained. This procedure is carried out for all ghost points to ensure that the desired boundary condition applies everywhere at the surface of the immersed object.

### 3. Results

In this section, we will present results obtained for the classical Graetz-Nusselt problem as well as an advanced Graetz-Nusselt problem simulated by using the CFM and DFM models. Sketch of the two geometries are shown in Fig. 1. The advanced Graetz-Nusselt problem is closely related to engineering applications and reveals the strong points of both IBM models in the application of heat transport processes in fluid-particle systems. In the first section, simulation results are compared with analytical solutions, which serves as a verification case of our two IBM models. Following that, the two IBM models are applied to a dense particle array positioned inside a tube with adiabatic wall. The influences of particle sizes and fractional amount of passive particles on the heat transfer performance are determined. For all the results, the two IBM models are compared, finding good agreement.

#### 3.1. Classical Graetz-Nusselt problem

The classical Graetz-Nusselt problem deals with forced heat convection combined with heat conduction of a fully developed laminar flow in an empty tube, see Fig. 1(a). It was first investigated by Graetz (1882) and Nusselt (1910) for the situation of a constant temperature (but different from the fluid inlet one) enforced at the wall of the tube. Later Tao (1961) and Tyagi (1966) extended this problem to the boundary condition of a constant heat flux, and provided a mathematical solution to that. The amount of heat transfer at the wall is defined as the ratio of convective to conductive heat transfer, which is commonly expressed by the Nusselt number $Nu$:

$$Nu = \frac{\alpha_0 D_f}{\lambda_f},$$

(18)

where $\alpha_0$ is the heat transfer coefficient, $D_f$ is the diameter of the tube and $\lambda_f$ is the thermal conductivity of the fluid.

The analytical solution for the constant wall temperature boundary condition is given by the following equation (Shah and London, 1978):

$$Nu_T = 3.6568 \left(1 + \frac{1.227}{Pe^{1/3}} + \cdots \right),$$

(19)

where $Pe$ is the Péclet number defined as:

$$Pe = Re Pr,$$

(20)

with Reynolds number $Re$ and Prandtl number $Pr$ respectively calculated as:

$$Re = \frac{\rho_f D_f \nu_f}{\mu_f},$$

(21)

$$Pr = \frac{C_p \mu_f}{\lambda_f}.$$  

(22)

For the case of a constant wall heat flux, the mathematical solution for the Nusselt number is a constant, namely (Shah and London, 1978):

$$Nu_{hi} = 48/11 = 4.36364.$$  

(23)

In our DNS, the fluid enters the tube with varying velocities, corresponding to Péclet numbers ranging from 5 to 100. The fluid inlet temperature is the same as the fluid initial temperature, and the data used for the simulations are summarized in Table 1. The Prandtl number is set to be unity, indicating the same thickness of the momentum and thermal boundary layers. The heat transfer coefficient is calculated as the heat flux divided by the driving force for the heat transfer process. For the case of a

![Fig. 1. Sketch for (a) classical Graetz-Nusselt problem and (b) advanced Graetz-Nusselt problem. In (a), fluid enters the tube at temperature $T_0$ and encounter the wall at a different fixed temperature or with a constant heat flux. In (b), a dense stationary particle array is added inside the tube which is adiabatic.](image-url)
constant wall temperature, the heat flux is averaged over the perimeter of the tube whereas the driving force is the difference between the prescribed wall temperature and the cup-average temperature of the fluid. For the case of a constant wall heat flux, the flux is a prescribed value and the driving force is computed as the difference of the averaged wall temperature and the cup-average temperature. The fluid cup-average temperature is calculated by the following equation:

$$\langle T_f \rangle = \frac{\int_S u(x,y,z)T_f(x,y,z)dydz}{\int_S u(x,y,z)dydz}.$$  \hspace{1cm} (24)

In this equation, the integration is performed over a surface $S$, perpendicular to the flow direction $x$, and $u(x,y,z)$ is the $x$ component of the fluid velocity at this certain point $(x,y,z)$.

Mesh convergence tests were first performed by using mesh resolution of 10, 20, 40 and 80, which is defined as the ratio of the tube diameter to the grid size. The tests were performed at $Pe = 30$ for both boundary conditions, and the simulation results are given in Fig. 2. It should be noted that the Nusselt number is computed at a location far beyond both the hydrodynamic and the thermal entrance regions (the tube length is 10 times $D_t$ and the Nusselt number is computed at the location of 9$D_t$). From the figure, good spatial convergence is observed for both boundary conditions. The convergence rate is 2 and 1.7 for DFM and CFM, respectively. CFM has a bit smaller convergence rate and larger deviations, which result from the nature of the smeared boundary treatment. Taking both accuracy and computational cost into consideration, mesh resolution 20 is selected for both DFM and CFM models.

The Nusselt numbers obtained from DNS are plotted as a function of the Péclet number in Fig. 3, comparing with the analytical solutions computed by Eqs. (19) and (23). As clearly demonstrated in the figure, compatible results are obtained from two IBM models for all Péclet numbers. For the case of a constant wall temperature $Nu_T$ decreases with larger $Pe$, which is due to the increased effect of the axial heat conduction in the fluid. For the constant heat flux boundary condition, $Nu_H$ is independent of $Pe$, which is an expected behavior as in this circumstance axial heat conduction is constant within the fluid. Additionally, the relative error between the IBM results and the analytical values and the relative deviation of the system energy balance are plotted in the figure for isothermal and isoflux boundary condition respectively. The profile of the relative error for the isoflux system has exactly the same trend as the profile of $Nu_H$, and the value is 0.67% and 1.14% for DFM and CFM respectively. The relative deviation of the system energy balance is calculated by Eq. (25), with energy inflow $Q_{h,in}$, energy outflow $Q_{h,out}$ and energy input from the tube wall $Q_{h,tube}$ computed by the next three equations:

$$Error = \frac{Q_{h,in} + Q_{h,tube} - Q_{h,out}}{Q_{h,tube}}.$$  \hspace{1cm} (25)

$$Q_{h,in} = \int_S \left( u_{in}T_{f,in}C_p\rho_f + \frac{q_{in}}{D_t} T_{f,in} - \frac{T_{f,1}}{dx} \right) dydz.$$  \hspace{1cm} (26)

$$Q_{h,out} = \int_S u_{out}T_{f,out}C_p\rho_f dydz.$$  \hspace{1cm} (27)

$$Q_{h,tube} = \pi D_t L_T.$$  \hspace{1cm} (28)

In $Q_{h,in}$ calculation $T_{f,1}$ is the fluid temperature at the first grid point in the flow direction, whereas in $Q_{h,tube}$ calculation $q$ and $L_T$ are the prescribed heat flux and the total length of the tube respectively. Through this test, we can conclude the excellent enforcement of both isothermal and isoflux boundary conditions at the wall of the tube. The simulation results are very accurate in the full $Pe$ range.

3.2. Advanced Graetz-Nusselt problem

In this section, we propose an advanced Graetz-Nusselt problem extended from the classical one by positioning a dense stationary particle array inside the tube, see Fig. 1(b). Both DFM and CFM models are applied to this physically more complex system containing a relatively large number of particles, and the simulation results obtained under varying conditions are analyzed and compared between these two models. In these simulations, fluid flows...
through a stationary random array of particles, and gets heated up at the surface of these particles. The particle array inside the tube is created by the hard-sphere Monte-Carlo method which considers both particle-particle collision and particle-tube collision, and distributed in a random configuration with a predefined solid phase packing density $\eta = 0.3$. The data used for the simulations are listed in Table 2. The simulations are computed on a 3D domain with the packing height of 0.1125 m and the diameter $D_T$ of 0.0375 m. It should be noted that in the simulations extra pipe lengths of 0.025 m and 0.075 m are reserved for inlet and outlet region, respectively, in order to avoid flow development and outflow recirculation problems, especially at high Reynolds numbers. For the simulations a prescribed uniform fluid velocity is imposed at the inlet, with the value of 0.32 m/s, 0.64 m/s and 0.96 m/s, corresponding to the tube based Reynolds numbers of 600, 1200 and 1800, respectively. At the inlet the fluid enters the tube with a uniform temperature which is the same as the initial temperature of the system. At the wall of the tube, no-slip boundary condition is applied to the velocity field computation whereas the tube is assumed to be adiabatic, i.e. a zero-flux Neumann boundary condition is applied for the temperature field computation.

In this advanced Graetz-Nusselt problem, a standard case (SC) is first set up by positioning 570 particles with the diameter $d_s$ of 0.005 m inside the tube. All spheres are active with the surface temperature 100 K higher than the fluid inlet temperature. Building on that, four extended cases are considered in two scenarios with the precondition of the same solid phase packing density $\eta = 0.3$. By changing particle size while keeping all particles active, the C1-1 case represents a binary mixture with 1:1 ratio of small particles ($d_s = 0.005$ m) and large particles ($d_s = 0.0075$ m), whereas there are only large particles in the C1-2 case. The particle Reynolds numbers based on particle radii with increasing velocities are 80, 160, 240 and 360 for small and large particles, respectively. In Fig. 4, the particle configurations for varying particle size are shown in both streamwise and radial directions. With the particle size ($d_s = 0.005$ m) unchanged, half of the particles in the array are passive, giving zero heating effect to the fluid phase, in the C2-1 case, and in the C2-2 case the array is further diluted by passive particles to 90%. The five cases with their features are listed in Table 3. Active particles might be hot catalysts which are heated up by the liberated heat from the exothermic reaction, while passive particles might be inert dilutions which are used to keep the system at a low conversion rate. The C1 cases are to study the influence of bidispersed particles, while the C2 cases are to study the thermal behavior of a diluted system. In this work, active particles are simulated by applying the Dirichlet boundary condition, whereas for passive particles the zero-flux Neumann boundary condition is imposed at the sphere surface. In all cases spheres are distributed in a random fashion. The mesh resolution, defined as the ratio of the particle diameter to the grid

通过一个静止的随机粒子阵列，以及在这些粒子的表面上被加热。粒子阵列在管子内创建，通过硬球Monte-Carlo方法考虑了粒子-粒子和粒子-管子碰撞，分布在随机配置中，具有预定义的固体相填充密度$\eta = 0.3$。用于模拟的数据列在表2中。模拟是在3D域上进行的，包含0.1125 m的填充高度和0.0375 m的直径$D_T$。重要的是，在模拟中在入口和出口区域保留额外的管道长度0.025 m和0.075 m，以避免流体发展和出流再循环问题，尤其是在高Reynolds数时。

在该先进的Graetz-Nusselt问题中，标准情况（SC）首先建立，放置570个直径为0.005 m的粒子在管内。所有粒子都是活跃的，表面温度比入口温度高100 K。在SC的基础上，考虑了四个扩展情况在两种场景中，前提是相同的固体相填充密度$\eta = 0.3$。通过改变粒子大小而保持所有粒子活跃，C1-1情况代表了大小粒子的二元混合物（1:1比），而C1-2情况仅含有大粒子。粒子Reynolds数是基于粒子半径的，随着速度的增加为80, 160, 240和360。在C2-1情况中，粒子大小（$d_s = 0.005$ m）不变，阵列中的一半粒子是被动的，对流体相没有加热效果。在C2-2情况中，阵列进一步稀释到90%的被动粒子。五种情况及其特征列在表3中。活性粒子可能是热催化剂，它们被热解反应中释放的热量加热，而被动粒子可能是惰性稀释剂，用于保持系统的低转化率。C1情况用于研究单分散粒子的影响，而C2情况用于研究稀释系统的热行为。在本工作中，活性粒子通过应用Dirichlet边界条件进行模拟，而对被动粒子应用零通量Neumann边界条件。

| 表2 | 用于先进Graetz-Nusselt问题的模拟数据。 |
| --- | --- | --- |
| 参数 | 值 | 单位 |
| 网格大小 | $2.5 \times 10^{-4}$ | m |
| 时间步长 | $5 \times 10^{-6}$ - $2 \times 10^{-5}$ | s |
| 液体密度 | 1 | kg/m³ |
| 液体粘度 | $2 \times 10^{-5}$ | kg/m/s |
| 液体比热容 | 1000 | J/kg/K |
| 液体热导率 | 0.02 | W/m/K |

| 图4 | 流向和径向方向的粒子配置，显示了小粒子、二元粒子和大粒子的分布（从左到右）。 |

| 表3 | 在先进Graetz-Nusselt问题中模拟的五种情况。 |
| --- | --- | --- | --- | --- |
| 代码 | 标准情况 | “大小”情况 | “被动”情况 |
| 总数 | 570 | 130+130 | 169 | 570 | 570 |
| 粒子直径（m） | 0.005 | 0.005+0.0075 | 0.0075 | 0.005 | 0.005 |
| 活跃粒子数 | 570 | 260 | 169 | 285 | 57 |

size, is 20 and 30 for small and large particle, respectively, in both DFM and CFM simulations. The same resolution was used for the numerical solution of the momentum and temperature equations, as $Pr = 1$. For DFM it was shown in an earlier publication that for this packing density and size ratio the used resolution suffices (Lu et al., 2018a). In CFM simulations, mesh convergence tests following the methodology in the aforementioned publication show that further increase of the grid resolution does not impact the results.

The velocity distribution is an important characteristic for the flow through a dense particle array positioned inside a tube. The highly irregular flow field has a significant influence on the heat transfer processes. Fig. 5 shows the averaged axial velocity profiles as a function of the dimensionless distance to the center of the tube for small, binary and large particle configurations at varying fluid velocities. The profile is obtained by: firstly dividing a transversal cross-section into a series of annuli with the thickness of the mesh size, secondly averaging the interstitial velocity at each radius and finally averaging the profiles of all transversal cross-sections along the length of the packing. As expected, the axial velocity profile is quite independent of the Reynolds numbers after nondimensionalization. The highest velocities are found close to the wall for all particle configurations, where the packing has its lowest densities. Locally an increase up to a factor of 3 is found for the small particle configuration, whereas this factor gradually decreases with more large spheres in the system. This factor matches well with the values in the range of 2.5–3.0 reported by Giese et al. (1998) and Eppinger et al. (2011). For larger particles, the lower fluid axial velocity in the near-wall region is compensated by higher and wider peaks of the fluid velocity inside the array, which is due to the decreased channeling effect in the near-wall region at reduced $D/d_t$ ratios. This is well described by the larger oscillating amplitude in the figure. The fluctuations of the radial dependence of the axial velocities reflect the variation of the local porosity. The profiles of two extreme cases (the SC case at $Re = 1800$ and the C1–2 case at $Re = 600$) are compared for CFM and DFM in Fig. 5 (c), which reveals excellent agreement. The computed velocity distributions, axial velocity and velocity magnitude for longitudinal and transversal cross-section respectively, at the Reynolds number of 1200 are shown in Fig. 6. The longitudinal cross-section is the central plane of the column, whereas the transversal cross-section locates at the height of 0.1 m in the particle array. In the figure preferred flow pathways can be clearly seen both inside the particle array and between the tube and the particles, with the former one becoming more pronounced at increased particle sizes. This corresponds well to the circumferential-averaged axial velocity profiles discussed before. In the longitudinal figures, negative values of the axial velocity indicating local back-mixing appear at the rear of the particles and at the end of the particle array. In the transversal figures, it is clearly demonstrated that the computed velocity field is zero inside the particles and outside the tube due to the particular enforcement of the no-slip boundary condition at the object surface.

For industrial application of tubular fluid-particle systems, the temperature profiles of the fluid phase in both streamwise and radial directions are of high interest. The streamwise profile is of significant importance for the temperature control during the production process, as continuously increasing temperature along the length of the reactor may result in damages of the catalyst. For this purpose, the cup-average temperature is computed and plotted along the domain length in Fig. 7. The calculation is already described in the previous section, namely Eq. (24). However, it must be emphasized here that for the array case only the part occupied by the fluid is accounted for in the integration of the profile.
cross-sectional surface and the value is further non-
dimensionalized by the particle temperature. In the figure, excel-
ten enforcement of the adiabatic tube, namely zero-flux Neumann boundary condition, can be clearly observed from the constant profiles in the outlet region. In the case of all spheres active, the fluid temperature rapidly increases in the front part of the array and slows down in latter parts due to the decreasing driving force for fluid-particle heat transfer, giving an exponential profile. With more large spheres in the system, the cup-average temperature profile has a slower increasing rate, although the solid phase fraction is the same. This is due to the smaller specific surface at increased particle sizes, leading to less fluid-solid contacting area. Regarding the influence of passive particles, as expected, the fluid is less heated by the particles which consequently leads to a lower temperature at the outlet. A nearly linear increase is observed in case of 90% dilution, which can be explained by the almost homogeneous heating in the full packing domain. Higher Reynolds numbers result in a lower heating effect between the particles and the fluid under any circumstance. The results obtained from CFM and DFM are in excellent agreement. CFM profiles are slightly higher than the DFM profiles, with only a few percent (maximal 3%) deviation. In Fig. 9 the temperature distributions for consents well with the velocity comparison, however with the deviation slightly amplified. In Fig. 9 the temperature distributions for the longitudinal and transversal cross-sections, but the influence is quite limited. Regarding the comparison between two models, it corre-
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Fig. 6. The computed velocity fields for small, binary and large particle configurations at Re = 1200 from DFM. Snapshots are shown for the central plane in the flow direction and the cross-section in the radial direction at the packing height of 0.1 m.

In this equation, \( T_i \) is the fixed particle temperature and \( \langle T_f \rangle \) is the cup-average temperature of the fluid phase in the current transversal cross-section. With that, the radial fluid temperature profile is produced applying the same method used in the axial velocity profile computation, namely the circumferential-averaged fluid temperature at each cross-section of the column is averaged along the full length of the packing. It should be noted that by using this definition with the minus sign in front of \( T_f \) the apparent change of \( T_f \) is actually opposite to the real change of \( T_p \). From the figure, large temperature differences are observed in all particles active case. The higher dimensionless temperature differences at the near-wall region result from the higher fluid velocities there. By position-
ing more large particles into the system, this difference is reduced to some extent with higher fluid temperature at the near-wall region and lower fluid temperature inside the packing. This agrees well with the previous velocity results, where it was shown that the channeling effect in the near-wall region is less for larger parti-
cles. By diluting with passive particles, the temperature difference is dramatically reduced. In other words, a more uniform tempera-
ture field is obtained radially in the fluid phase if the particle array consists of fewer active particles. Increasing the Reynolds number always contributes to a more uniform distribution of the tempera-
ture field in the transversal cross-sections, but the influence is quite limited. Regarding the comparison between two models, it corre-
sponds well with the velocity comparison, however with the deviation slightly amplified. In Fig. 9 the temperature distributions for the longitudinal and transversal cross-sections, but the influence is quite limited. Regarding the comparison between two models, it corre-

in Fig. 8. Due to the con-
tinuous rise of the fluid temperature in the flow direction, a dimen-
sionless temperature is defined so that it can be averaged over axial positions:

\[
\bar{T}_f = \frac{T_s - T_f}{T_s - \langle T_f \rangle}.
\] (29)

The reactor-based heat transfer coefficient \( \alpha_{h,\text{reactor}} \) is computed to evaluate the overall heat transfer performance of the reactor, which is defined as:

\[
\alpha_{h,\text{reactor}} = \frac{Q_h}{A_{\text{total}} \Delta T}.
\] (30)
In this equation, $A_{\text{total}}$ is the total surface area of all active particles. The total amount of heat transferred is computed by selecting two transversal cross-sections at the two ends of the column:

$$Q_h = Q_{h,\text{out}} - Q_{h,\text{in}} = C_{ff} \rho_f \int \left[ u_{\text{out}}(y,z) T_{f,\text{out}}(y,z) - u_{\text{in}}(y,z) T_{f,\text{in}}(y,z) \right] dy dz,$$

and the overall heat transfer driving force is calculated as the logarithmic mean temperature (Das et al., 2017a):

$$\Delta T = \frac{\Delta T_{f,\text{in}} - \Delta T_{f,\text{out}}}{\ln \frac{M_{\text{in}}}{M_{\text{out}}}}.$$

$$\Delta T_{f,\text{in}} = T_s - T_{f,\text{in}},$$

$$\Delta T_{f,\text{out}} = T_s - T_{f,\text{out}}.$$

It should be noted, although a dimensionless fashion of the heat transfer coefficient, i.e.: Nusselt number defined by the following equation using characteristic length $L_c$ and thermal conductivity $\lambda_f$, is more general for engineering applications,

$$Nu = \frac{a_{h,\text{reactor}} L_c}{\lambda_f},$$

we consider a case with binary particle sizes for which the choice of $L_c$ is ambiguous, and hence we prefer to use the dimensional (but consistent) heat transfer coefficient to avoid introducing further debate regarding the equivalent diameter. The computed reactor-based heat transfer coefficient $a_{h,\text{reactor}}$ is plotted in Fig. 10, with simultaneous comparison between the DFM results and the CFM results. To date there is no empirical correlation proposed for heat transfer processes matching our physical model in current work, as it is of high difficulty to measure heat transfer data under such complex circumstances experimentally. In particular, the adiabatic tube wall and the small ratio of tube to sphere diameter are parameters having strong influences on the heat transfer processes, which are however not addressed conjointly in literature. We consider our
Fig. 8. Circumferential-averaged fluid temperature profiles as a function of the normalized distance to the tube center. The influence of varying particle sizes is presented in top panels ((a) from DFM, (b) from CFM) and the influence of passive particles dilution is presented in middle panels ((c) from DFM, (d) from CFM). Same legends are applied for CFM and DFM. The comparison of two selected cases between CFM and DFM are presented in bottom panels ((e) for “size” scenario, (f) for “passive” scenario).

Fig. 9. Temperature distribution of all cases at Re = 1800 from DFM, for the central plane in the flow direction and the cross-section at the packing height of 0.1 m.

results as the first step towards the assessment of the effect of varying particle conditions (size and dilution) on the heat transfer processes in adiabatic tubular systems, especially with the non-negligible wall effect. The insights revealed from numerical studies are highly reliable, as consistent results are obtained from two IBM models which have been verified in previous publications (Lu et al., 2018a,b; Uhlmann, 2005; Fadlun et al., 2000). In Fig. 10, the values obtained from the empirical Gunn correlation for the SC case are also plotted as reference. Regarding the wall effect, although the heat transfer performance is improved to some extent at higher fluid velocities at the near-wall region, the strong channeling significantly reduces the overall heat transfer efficiency providing the fact that all cases with all spheres active have much lower values than the empirical ones predicted by the Gunn correlation. Comparing to studies applying the periodic boundary condition in spanwise directions (Tavassoli et al., 2013; Sun et al., 2015; Municchi and Radl, 2017), where computed and empirical heat transfer coefficients were much closer, the channeling effect at the near-wall region is clearly illustrated. It might be unexpected to see an increase of the reactor-based heat transfer coefficient by positioning larger particles in the system, as in this case the ratio of tube to sphere diameter is smaller and consequently the wall effect should be larger. However, as clearly visualized in Figs. 6, 8 and 9, for these larger particles the near-wall channeling effect is less. The increase by diluting with passive particles is due to the dramatically improved local heat transfer driving force between the particle temperature and the surrounding fluid temperature. Considerably lower fluid temperatures were already illustrated in Figs. 7 and 9. As forced convection is the main mechanism for heat transfer in the current model, the reactor-based heat transfer coefficient

Fig. 10. The reactor-based heat transfer coefficient obtained from two IBM models, for all five cases with varying fluid velocities. DFM results are presented in panel (a), whereas CFM results are presented in panel (b). Same legends are applied for CFM and DFM.

Fig. 11. The profile of the slice-based heat transfer coefficient at the Reynolds number of 1200, along the normalized length in the flow direction. The influence of varying particle sizes is presented in top panels ((a) from DFM, (b) from CFM), and the influence of passive particles dilution is presented in bottom panels ((c) from DFM, (d) from CFM). Same legends are applied for CFM and DFM.
increases with higher Reynolds numbers. The two IBMs give very similar results, with less than 8% deviation. The reactor-based heat transfer coefficients obtained from the CFM are always higher than the ones given by the DFM, and this corresponds well with what we had observed for the fluid temperature which we discussed before.

Next, the slice-based heat transfer coefficient $a_{h,slice}$ is computed to describe the spatial distribution of the local heat transfer coefficient in the surface perpendicular to the flow direction, using the following equation:

$$a_{h,slice} = \frac{\nabla T_f \cdot \bar{n}}{\frac{T_s}{C_1} / \frac{T_f}{C_10/C_11} k_f (\bar{T}_f)^3}$$

where $\nabla T_f \cdot \bar{n}$ is the average temperature gradient at the particle surface for all particle sections located in the current slice, and the cup-average temperature of the fluid phase at this particular cross-section is used for calculating the local driving force. In the calculation only the sections of active particles are considered in the average. The slice-based heat transfer coefficients $a_{h,slice}$ obtained from our simulations are plotted in Fig. 11 along the flow direction, for the case of the Reynolds number of 1200. As expected, fluctuations of the slice-based heat transfer coefficient are observed in the full packing zone along the flow direction, which is mainly due to the variation of the fluid-particle interface in the cross-sections. In top panels, namely undiluted cases, entrance and outlet regions are clearly observed inside the bed. With varying particle sizes, there is no distinct difference in the length of the entrance region, which is approximately $L_e/L_T = 0.3$. The large entrance effect is due to the simultaneous effect from both the bulk and the near-wall region, whereas later the bulk is thermally saturated and only the near-wall region contributes to the heat transfer. This point will be further revealed in the next paragraph. The length of the outlet region is much shorter comparing to that of the entrance region, and it seems to be further reduced at larger particle sizes. A region in the middle of the packing, namely between the entrance and the outlet regions, has the slice-based heat transfer coefficients

Fig. 12. Radial distribution of the particle-based heat transfer coefficient for the SC case at three Reynolds numbers. All individual values with the particles in the entrance region indicated by open circles are presented in panel (a) (DFM) and (c) (CFM). The average values with error bar computed by excluding particles in the entrance region are presented in panel (b) (DFM) and (d) (CFM). Same legends are applied for CFM and DFM. A parity plot between CFM and DFM results at $Re = 600$ is shown in panel (e).
fluctuating around a constant value and the amplitude is enlarged to some extent with larger particle sizes. In bottom panels, the system is diluted by passive particles and the profiles behave considerably different. With less active particles in the system, the profile of the slice-based heat transfer coefficient rises due to the less thermal saturation in the fluid phase. With half of the particles passive, the entrance effect acts over a much longer length with a much slower decay rate, comparing to the one of the SC case. No clear “constant” region is observed anymore. If the system is further diluted to only 10% active particles, the profile does not clearly show a “decay” shape, as the entrance length is so long that only the entrance behavior is visualized. It should be noted that the variation of the fluid-particle interface in the previous C1 cases is due to the local varying porosity, while in the C2 cases, where the packing structure is unchanged, it is due to the varying surface area of active particles contacting with the fluid. Reasonably, due to the less even spatial distribution of the active fluid-particle interface, the fluctuation amplitude increases dramatically with more passive particles in the system. The slice-based heat transfer coefficients at the Reynolds number of 600 and 1800 have very similar behavior with the ones discussed here, with the corresponding profiles lower and higher respectively. DFM results and CFM results are in good agreement. Similar to the reactor-based heat transfer coefficient, the profiles of the slice-based heat transfer coefficient obtained from the CFM are a bit higher in the full packing zone than the ones obtained from the DFM. At the same time, the oscillation frequencies are quite close, but the amplitudes are always larger in CFM results which is a consequence of the discrete nature of the Lagrangian points on the particle surface.

Taking the advantage that all detailed information can be obtained from DNS, we are interested to go to the bottom level to evaluate the heat transfer performance of individual particles. For this purpose, the particle-based heat transfer coefficient $\alpha_{\text{h, particle}}$ is defined by the following expression:

$$\alpha_{\text{h, particle}} = \frac{\Phi_{\text{h,s-f}}}{4\pi r_i^2 (T_s - \left< T_s \right>)},$$

where $\Phi_{\text{h,s-f}}$ is the heat transfer rate, with the normal pointing outward of the solid. This quantity is calculated by the integration of the temperature gradient at particle surface over the whole particle (with $A_s$ of the particle external surface area):

$$\Phi_{\text{h,s-f}} = \int_{A_s} (-\kappa_s \nabla T_s \cdot n) dA_s.$$  

For passive particles, this quantity automatically goes to zero. The fluid cup-average temperature of the transversal cross-section at the sphere center is used for the local driving force calculation. In Fig. 12, the radial distributions of the particle-based heat transfer coefficient $\alpha_{\text{h, particle}}$ for the SC case are shown at different fluid velocities. In the distribution containing all individual values (panel (a) and (c)), a distinct group of data points indicating a ring-like structure is observed near the wall. Besides the ones at the outer shell, it is noticed that a considerable amount of particles inside the array also has large heat transfer coefficients. To understand the reason behind these high values, the particles in the entrance region are indicated by open circles whereas the remaining particles are indicated by closed circles. From the figures, it is clearly identified that large heat transfer coefficients inside the array dominantly originate from the particles in the entrance region. There are few closed circles with higher values, and simultaneously few open circles are inside the margin of closed circles. This can be explained by the property of...
the porous medium that preferred fluid pathways exist inside the particle array. Higher heat transfer coefficients are obtained for all particles at higher Reynolds numbers, but the improved amount strongly depends on the local flow structure (namely local particle distribution). The average values of the particle-based heat transfer coefficients are plotted with the radial position in panel (b) and (d), obtained from DFM and CFM results, respectively. It should be noted that only particles behind the entrance region are used for the calculation. As indicated in the figures, the particle-based heat transfer coefficient decreases from the outer shell to the array center, which is due to the high fluid velocities at the near-wall region. At higher Reynolds numbers, the profile rises with simultaneously increased fluctuations and error bars. This is due to the increased heterogeneity of the flow field. Qualitatively, very good agreement is reached between CFM and DFM results. Based on the earlier discussions, we already expect higher values of the CFM results, which are clearly demonstrated by both individual and average values. To offer a more clear comparison, a parity plot between CFM and DFM results at the Reynolds number of 600 is shown in panel (e). Besides the confirmation of the preceding finding, the figure further reveals wider scatters and larger deviations at higher particle-based heat transfer coefficients.

With larger particles in the array, the outer ring of the particles still aligns with the tube wall. In other words, if we plot a figure like Fig. 12(a) or (c), two groups of outer-ring particles would be observed in the C1-1 case, which correspond to the small particle and large particle location in the SC and C1-2 case, respectively. In Fig. 13, the influence of larger particles on the particle-based heat transfer coefficient is shown. The average values with error bars, computed by excluding the particles in the entrance region, are plotted in the radial direction at the Reynolds number of 1800. The average particle-based heat transfer coefficient decreases from outer to inner shells regardless of the tube-to-particle diameter ratio. It should be noted, the abnormal behavior for the C1-2 case at the outer shell is due to insufficient statistical data. With more large particles, the heat transfer coefficients inside the array increase considerably. Besides that, the error bar of particles inside the array becomes larger, as the flow field is more heterogeneous at larger particle sizes. A parity plot is made to give an impression of the deviation between CFM and DFM results for all individual particle-based heat transfer coefficients in the C1-2 case, which shows consistent behavior with the SC case.

The influence of passive particles on the particle-based heat transfer coefficient is shown in Fig. 14, at the Reynolds number of 1800. Due to the significantly increased length of the entrance region, all particles are plotted without any distinction. In panel (a) and (c), where the individual particle-based heat transfer coefficients are plotted radially, they are more homogeneously distributed in the systems diluted by passive particles. In the C2-1 case, a decrease from the outer ring to inner particles is still identifiable, however with a much diffusive distribution for “bottom” values. In the C2-2 case, this wall-enhanced distribution completely disappears such that all active particles have relatively high heat transfer coefficients regardless of their radial positions. In the right panels ((b) and (d)), the heat transfer coefficient of individual particle in diluted systems is plotted with its value in the SC case. In other words, the dilution effect can be revealed by comparing the heat transfer coefficient of the same particle. In the C2-1 case, namely the system diluted by 50% passive particles, a rough linear distribution with diffusive upper boundary can be observed, which indicates the limited enhancement of the heat transfer performance of active particles by passive particles (i.e.: fluid flow dominates the heat transfer behavior). By further dilution, namely the C2-2 case, the significant (dominating) effect of the surrounding...
passive particles can be identified that the heat transfer coefficients of all active particles are randomly distributed in a narrow range, regardless of their values in the SC case.

4. Conclusions and outlook

In this paper, CFM and DFM, which are the two categories of IBMs, are applied to perform DNS simulations of heat transfer problems in tubular fluid–particle systems. These two models are both extended from the well-developed momentum transfer models to handle heat transfer, and are applied to identical physical systems to offer an efficient comparison. Both of our methods have the capability to handle mixed boundary conditions at the immersed object surface. To be specific, the isothermal and insulox boundary conditions, which are widely encountered in industrial processes, are enforced in our DNS work. In all simulations, excellent agreement are reached between CFM and DFM results, with the deviation being below 10%. Considering the nature of capturing the discontinuity at the fluid-solid interface, DFM might offer a more accurate result, which however requires more follow-up simulations to give a solid investigation. Due to the Lagrangian points and the delta function applied in CFM, the temperature distributions are smoother but the heat transfer coefficients have larger oscillations. Regarding the computational efficiency, there is no substantial difference between these two methods.

In the classical Graetz-Nusselt problem, our simulation results are verified to excellently match the analytical solutions. In the advanced Graetz-Nusselt problem, namely a dense stationary array consisting of hundreds of particles randomly positioned inside a tube with adiabatic wall, the influence of particle size, passive particles and the Reynolds number are studied. With larger particles, the fluid velocity profile has stronger oscillations inside the particle array, indicating a more heterogeneous flow field, and the reactor-based, slice-based as well as the particle-based heat transfer coefficients are larger. With passive particles, a more uniform fluid temperature field is obtained in the transversal cross-sections and the reactor-based heat transfer coefficient is dramatically increased. The slice-based heat transfer coefficient is increased too, but with more pronounced oscillations, whereas the heat transfer coefficients of individual particles are more homogeneously distributed in a narrower range with higher values. Higher Reynolds number will improve the heat transfer performance under any circumstance.

As future work, it is interesting to perform intensive parameter study, varying more parameters such as the Reynolds number, the Prandtl number, the solid phase packing density, the tube-to-particle diameter ratio, the passive particles dilution ratio and the ratio of bidispersed or even polydispersed particles. Such simulations will reveal insight into the influence of these practically relevant parameters. The two IBM models can be mutually corroborated to give convincing and reliable results. Using the detailed information provided by such simulations, hopefully, a “Gunn-like” empirical correlation could be proposed to characterize the fluid-particle interfacial heat transfer in tubular systems.

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