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Corresponding Author: Dr. Shankar Subramaniam, Ph.D.

Corresponding Author's Institution: Iowa State University

First Author: Sudheer Tenneti

Order of Authors: Sudheer Tenneti; Bo Sun; Rahul Garg, PhD; Shankar Subramaniam, Ph.D.

Abstract: Heat transfer is important in gas--solid flows that are encountered in many industrial applications such as energy generation. Computational fluid dynamics (CFD) simulations of heat transfer in gas-solid flow are based on statistical theories that result in averaged equations (eg., Eulerian-Eulerian two-fluid model). These averaged equations require accurate models for unclosed terms such as the average gas-solid heat flux. The average gas-solid or interphase heat flux is closed in terms of the Nusselt number Nu , which is specified as a function of the solid volume fraction ϵ , mean flow Reynolds number Re and Prandtl number Pr . In developing closure models for the average interphase heat flux it is assumed that the gas-solid flow is locally homogeneous i.e., the effect of fluid heating (or cooling) on the average fluid temperature is neglected. However, continuous heating (or cooling) of the fluid along the flow direction causes the average fluid temperature to become inhomogeneous. In this work we develop a particle-resolved direct numerical simulation (PR-DNS) methodology to study heat transfer in steady flow past statistically homogeneous random assemblies of stationary particles. By using an analogy with thermally fully developed flow in pipes, we develop a thermal similarity condition that ensures a statistically homogeneous Nusselt number, even though the average fluid temperature field is inhomogeneous. From PR-DNS results we find that the effect of fluid heating cannot be neglected for gas-solid systems with high solid volume fractions and low mean flow Reynolds numbers. These results indicate that the assumption of scale separation implicit in two-fluid models is not always valid.

095E, H. M. Black Engineering Building
Department of Mechanical Engineering
Iowa State University
Ames, IA 50011
Ph: (515) 294-0369
Fax: (515) 294-3261
email: sudheert@iastate.edu

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This is previously unpublished work and has not been simultaneously submitted for publication elsewhere. Thank you.

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S. Tenneti
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S. Subramaniam

Role of fluid heating in dense gas–solid flow as revealed by particle–resolved direct numerical simulation

S. Tenneti^a, B. Sun^a, R. Garg^a, S. Subramaniam^{a,*}

^a*Department of Mechanical Engineering, Center for Computational Thermal–fluids Research, Iowa State University, Ames, IA 50011, USA*

Abstract

Heat transfer is important in gas–solid flows that are encountered in many industrial applications such as energy generation. Computational fluid dynamics (CFD) simulations of heat transfer in gas–solid flow are based on statistical theories that result in averaged equations (eg., Eulerian–Eulerian two–fluid model). These averaged equations require accurate models for unclosed terms such as the average gas–solid heat flux. The average gas–solid or interphase heat flux is closed in terms of the Nusselt number Nu , which is specified as a function of the solid volume fraction ε_s , mean flow Reynolds number Re_m and Prandtl number Pr . In developing closure models for the average interphase heat flux it is assumed that the gas–solid flow is locally homogeneous i.e., the effect of fluid heating (or cooling) on the average fluid temperature is neglected. However, continuous heating (or cooling) of the fluid along the flow direction causes the average fluid temperature to become inhomogeneous. In this work we develop a particle–resolved direct numerical simulation (PR–DNS) methodology to study heat transfer in steady flow

*Corresponding author

Email address: shankar@iastate.edu (S. Subramaniam)

past statistically homogeneous random assemblies of stationary particles. By using an analogy with thermally fully developed flow in pipes, we develop a thermal similarity condition that ensures a statistically homogeneous Nusselt number, even though the average fluid temperature field is inhomogeneous. From PR-DNS results we find that the effect of fluid heating cannot be neglected for gas-solid systems with high solid volume fractions and low mean flow Reynolds numbers. These results indicate that the assumption of scale separation implicit in two-fluid models is not always valid.

1. Introduction

Gas-solid flows occur in many industrial applications such as energy generation, food, chemical, and pharmaceutical processing. Carbon-neutral energy generation using biomass (Azar et al., 2006) or chemical looping combustion (Shen et al., 2008) (CLC), and CO₂ capture from flue gases using dry sorbents (Yi et al., 2007; Abanades et al., 2004) are examples of emerging technologies (Wall, 2007) where an improved understanding of gas-solid heat transfer is crucial for process and component design. For instance, accurate prediction of the fluid-phase temperature field is very important for the CLC application because the reaction rates in combustion chemistry are highly temperature dependent. Similarly, in the CO₂ capture process using potassium-based dry sorbents the carbonation reaction is exothermic and the regeneration of the sorbent is endothermic (Yi et al., 2007). Hence, gas-solid heat transfer is crucial for maximizing process efficiency. Both CLC and CO₂ capture technologies can be implemented using fluidized beds, and typical particle diameter values range from 50–150 μm . These particles are

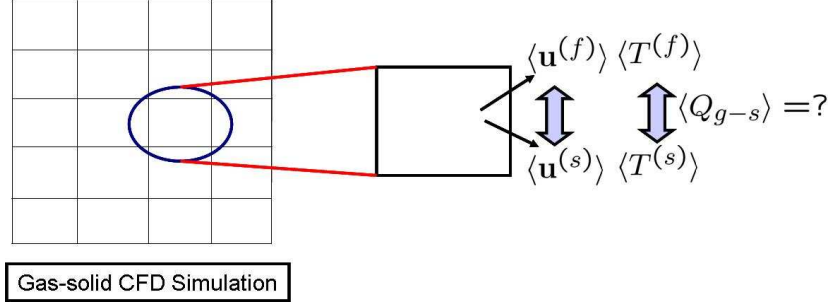


Figure 1: Schematic of a CFD simulation of gas–solid flow. In every computational grid cell, governing equations for the averaged quantities in both phases are solved. Here, $\langle \mathbf{u}^{(f)} \rangle$ is the average fluid–phase velocity, $\langle T^{(f)} \rangle$ is the average fluid–phase temperature, $\langle \mathbf{u}^{(s)} \rangle$ is the average solid–phase velocity and $\langle T^{(s)} \rangle$ is the average solid–phase temperature. In this schematic, $\langle Q_{g-s} \rangle$ denotes the average gas–solid interphase heat transfer.

typically larger than the Kolmogorov length scale of turbulent dissipation η . Moreover, gas–solid flow in fluidized beds can have a solid volume fraction ranging from near close–packed (64% for random configurations of monodisperse spheres) to as low as 5% in the riser region. A fundamental understanding of heat transfer in fluid flow past finite sized particles ($D > \eta$) over a wide range of solid volume fraction and flow Reynolds number is therefore important for process design.

Computational fluid dynamics (CFD) simulations (Syamlal et al., 1993; Kashiwa and Gaffney, 2003; Sun et al., 2007) of gas–solid flow are increasingly being used as an efficient approach for design optimization because experiments are often costly and time-consuming. In two–fluid CFD simulations of gas–solid flow, the averaged equations governing mass, momentum, and energy conservation are solved. Figure 1 shows a schematic of the computational domain in a CFD simulation of gas–solid flow. In every grid cell,

governing equations for averaged quantities such as volume fraction, velocity and temperature are solved for both phases. Since these equations are obtained using a statistical averaging procedure (Anderson and Jackson, 1967; Drew and Passman, 1998), the average interaction terms corresponding to mass, momentum, and energy exchange between different phases need to be modeled. For example, two-fluid CFD formulations for heat transfer in gas-solid flow require closure of the average gas-solid heat transfer $\langle Q_{g-s} \rangle$. The average interphase heat flux $\langle Q_{g-s} \rangle$ is modeled in terms of an average Nusselt number and the difference between the average fluid and solid-phase temperature ($\langle T^{(f)} \rangle - \langle T^{(s)} \rangle$). This Nusselt number is usually given by a correlation that depends on solid volume fraction ε_s , mean slip Reynolds number Re_m and the Prandtl number Pr .

Correlations for the Nusselt number corresponding to gas-solid heat transfer are typically obtained from a combination of experimental and theoretical studies. However, the experimental data from which these empirical correlations are deduced vary by orders of magnitude (Wakao and Kaguei, 1982; Breault and Guenther, 2009). Experimental measurement of heat transfer in gas-solid flow is challenging because of limited optical access and hence most measurements are intrusive. Theoretical studies of heat transfer in gas-solid systems are limited to creeping flow past ordered (Pfeffer and Happel, 1964; Sorensen and Stewart, 1974) and random assemblies of spheres (Gunn, 1978; Acrivos et al., 1980). The randomness in particle positions and velocities together with the nonlinearity of the governing equations make the analytical treatment intractable at finite Reynolds numbers. Particle-resolved direct numerical simulation (PR-DNS) of heat transfer in gas-solid flow is

a first-principles, model-free simulation method that can be used to gain better understanding of heat transfer in gas-solid flow. Furthermore, PR-DNS can be used to specify closure models for the unclosed average interphase interaction terms that arise in CFD simulations of gas-solid flow.

In applying closure models for the average interphase interaction terms such as the average interphase momentum transfer and interphase heat flux, it is assumed that the gas-solid flow is locally homogeneous. In other words, the average fluid and solid-phase velocities and temperatures are assumed to be uniform in the grid cell. Therefore, in order to specify closure models for the unclosed terms it is natural to simulate a statistically homogeneous gas-solid suspension using PR-DNS. Indeed, PR-DNS has been used successfully to solve the hydrodynamic problem and to provide a closure model for the average gas-solid momentum transfer. The closure for the average interphase momentum transfer is popularly known as a “drag law” and several researchers have extracted computational drag correlations for gas-solid flow by simulating steady flow past statistically homogeneous random assemblies of stationary spherical particles (Hill et al., 2001a,b; van der Hoef et al., 2005; Beetstra et al., 2007; Yin and Sundaresan, 2009a,b; Holloway et al., 2010; Tenneti et al., 2011) in periodic domains. Tenneti et al. (2011) have rigorously shown that the evolution equation for the volume averaged fluid-phase momentum obtained from this setup is consistent with statistically homogeneous ensemble-averaged equations. This problem setup ensures that the flow field is statistically homogeneous and statistics such as the average interphase momentum transfer can be easily obtained by volume averaging.

In the heat transfer problem, the assumption of a statistically homoge-

neous average fluid temperature implies that the effect of heating (or cooling) by the particles does not change the average fluid temperature significantly. However, continuous heating (or cooling) of the fluid by the particles along the flow direction can cause the average fluid temperature to vary in that direction. The extent of this variation of the average fluid temperature depends on the solid volume fraction and mean flow Reynolds number. Although the hydrodynamic problem is *statistically homogeneous*, for some regimes of gas–solid flow it is conceivable that anisotropy in the fluid velocity results in a *statistically inhomogeneous* fluid temperature field. Therefore, PR–DNS methodologies that are used to specify a closure model for the average Nusselt number in terms of the average solid volume fraction and mean flow Reynolds number must account for this inhomogeneity in the fluid temperature field. In this work we present a PR–DNS methodology to study heat transfer in statistically homogeneous gas–solid flow in periodic domains that accounts for the inhomogeneity in the temperature field. We use the analogy of flow in a fixed bed of particles with thermally fully developed flow in internal pipes to develop a thermal similarity condition that guarantees a statistically homogeneous Nusselt number. Using this new formulation we examine the regime of validity of the assumption of statistical homogeneity in the average fluid temperature field that is implicit in two–fluid CFD models.

We use the Particle–resolved Uncontaminated–fluid Reconcilable Immersed Boundary Method (PReIBM) (Garg et al., 2010b; Tenneti et al., 2010, 2011) to solve for heat transfer in gas–solid flow. We employ three–dimensional Cartesian grids to solve for the velocity, pressure, as well as the temperature fields. Dirichlet boundary conditions for both velocity and temperature at

the surface of the particle are imposed via an immersed boundary (IB) forcing that is added to the momentum and temperature equations, respectively. The idea behind the extension of the IB method to the temperature equation is similar to the one used by Feng and Michaelides (2008) to study heat transfer in particle-laden flow with solid to fluid density ratio in the range 1.001–1.1.

The rest of the paper is organized as follows. The problem description and the assumptions made to simplify the problem are described in section 2. The formulation of the heat transfer problem that is simulated in the particle-resolved DNS methodology is discussed in section 3. The governing equations are developed in section 4 and the numerical method used in our PR-DNS approach is described in section 5. The results obtained from PR-DNS of heat transfer in gas-solid flow are discussed in section 6 and finally the principal conclusions of this work are summarized in section 7.

2. Problem description

A schematic of the problem setup that is used in this work to study gas-solid heat transfer in a homogeneous suspension of randomly distributed spherical particles is shown in Fig. 2. The figure shows a random assembly of spherical particles in a unit cell, which repeats infinitely in all three directions. A steady flow is established by imposing a mean pressure gradient that corresponds to a mean flow Reynolds number that is defined based on the magnitude of mean slip velocity between the two phases as follows:

$$\text{Re}_m = \frac{|\langle \mathbf{W} \rangle| (1 - \varepsilon_s) D}{\nu_f}. \quad (1)$$

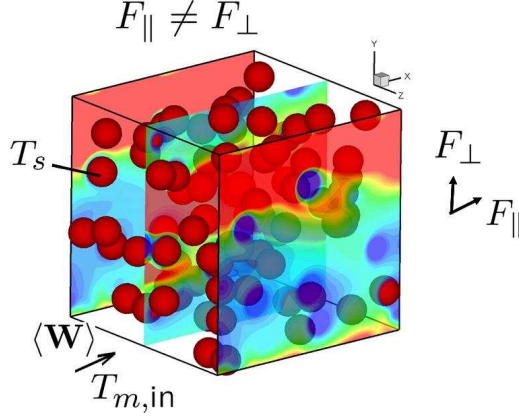


Figure 2: Schematic showing contours of steady temperature field in a flow through fixed bed of particles (solid volume fraction 0.1 and Reynolds number 20). In this schematic, $\langle \mathbf{W} \rangle$ is the mean slip velocity between the solid and the fluid-phase. The fluid enters the domain at a bulk temperature of $T_{m,in}$ and all the particles are held at a uniform constant temperature T_s .

Here $|\langle \mathbf{W} \rangle|$ is the magnitude of the mean slip velocity between the solid and fluid phases, which is in the direction shown in Fig. 2, D is the particle diameter and ν_f is the kinematic viscosity of the fluid. The bulk temperature of the fluid at the “inlet” of this unit cell is $T_{m,in}$ and all the particles are held at a uniform constant temperature of T_s . The bulk temperature of the fluid is the flux-weighted average temperature in a plane perpendicular to the direction of the mean slip velocity (see section 3 for a detailed definition). The difference in the bulk fluid temperature and the surface temperature of the particle drives gas-solid heat transfer. Here we consider only gas-solid flow so the Prandtl number is chosen to be 0.72. We neglect viscous heating, radiation and the effect of temperature change on the momentum equation due to density variation (free convection effects). The simplifying

assumptions used in our problem setup are justified in Appendix A. We now develop a formulation that can be used to study the gas–solid flow heat transfer problem described in this section.

3. Formulation of the heat transfer problem

In order to use the problem setup shown in Fig. 2 to quantify the average Nusselt number, we must ensure that the heat transfer problem admits a statistically homogeneous Nusselt number. In other words, a thermally fully developed flow must be established in the fixed bed. Flow through a fixed bed of spheres is anisotropic due to finite mean slip velocity $\langle \mathbf{W} \rangle$ between the solid and fluid phases. This directionality in the flow implies that fluid downstream of a particle is heated up (or cooled down) by interphase heat transfer. This continuous heating of the fluid by the particles results in a mean fluid temperature that is inhomogeneous (Acrivos et al., 1980) in the coordinate directed along the mean flow. However, since Nusselt number is a nondimensional interphase heat flux, if the driving force (temperature difference between bulk fluid and particles) has the same variation as that of the interphase heat flux along the flow coordinate, it is possible to obtain a statistically homogeneous Nusselt number. In this section we develop a formulation that renders the Nusselt number statistically homogeneous, although the interphase heat flux and the mean fluid temperature are inhomogeneous.

In order to understand the heat transfer problem in statistically homogeneous suspensions we draw analogy from forced convection heat transfer in internal pipe flow. Statistically homogeneous gas–solid flow is analogous

to fully developed pipe flow in two respects. Firstly, the flow field is statistically axisymmetric (Tenneti et al., 2012), similar to the fully developed flow field in a pipe. Secondly, the *average* area occupied by the fluid (or the area fraction) in any plane perpendicular to the streamwise direction is constant in a statistically homogeneous suspension, and hence can be compared to a pipe with a constant area of cross section. Therefore, in an *average* sense we expect the heat transfer problem in statistically homogeneous gas–solid suspensions with isothermal particles to be similar to thermally fully developed flow in pipes with isothermal walls. For internal pipe flow, the flow is said to be thermally fully developed when the scaled temperature is not varying in the streamwise direction (Incropera et al., 2006), i.e.,

$$\frac{\partial}{\partial x} \left(\frac{T(\mathbf{x}, t) - T_w}{T_m(x, t) - T_w} \right) = 0. \quad (2)$$

Without loss of generality we will assume that the flow direction is along the x -axis. In the definition of the scaled temperature given above, T_w is the temperature of the isothermal pipe wall and T_m is called the “mixing-cup” or “bulk” temperature, which is defined as follows:

$$T_m(x) = \frac{\int_{A_f} (\mathbf{u}T) \cdot \mathbf{e}_{\parallel} dA_f}{\int_{A_f} \mathbf{u} \cdot \mathbf{e}_{\parallel} dA_f} \quad (3)$$

where \mathbf{e}_{\parallel} is the unit vector along the streamwise direction and A_f is the area occupied by the fluid in a plane perpendicular to the streamwise direction. The thermally fully developed condition implies that for a pipe with constant cross-sectional area and isothermal walls, the local heat transfer coefficient at the wall (or Nusselt number) is independent of axial location (Incropera et al., 2006). In other words, the local wall heat flux scaled by the temperature difference ($T_m(x) - T_w$) is a constant. By using an analogy with pipe

flow, the average Nusselt number in gas–solid flow will be statistically homogeneous if we ensure that the scaled temperature field θ , which is defined below is statistically homogeneous:

$$\theta(\mathbf{x}, t) = \frac{T(\mathbf{x}, t) - T_s}{\langle T_m \rangle(x, t) - T_s}. \quad (4)$$

In this definition, $\langle T_m \rangle(x, t)$ is the ensemble-averaged bulk temperature and T_s is the uniform temperature at which all the particles are maintained. In the next section we discuss the governing equations and boundary conditions for the problem of heat transfer past stationary isothermal particles in periodic domains that ensure that the normalized interphase heat flux is statistically homogeneous.

4. Governing Equations

The fluid temperature field $T(\mathbf{x}, t)$, in the absence of viscous heating, radiation and free convection effects, obeys the following convection–diffusion equation:

$$\frac{\partial T}{\partial t} + \frac{\partial(u_j T)}{\partial x_j} = \alpha_f \frac{\partial^2 T}{\partial x_j \partial x_j}, \quad (5)$$

where $\alpha_f = k_f / (\rho_f C_{pf})$. Here k_f is the thermal conductivity, ρ_f is the thermodynamic density, and C_{pf} is the heat capacity of the fluid respectively. Equation (5) needs to be solved in the fluid together with the Dirichlet boundary condition of $T = T_s$ at the surface of the particles. At the boundaries of the computational domain, periodic boundary conditions are applied on the *scaled temperature* θ (cf. Eq. 4). In the definition of θ for a random particle assembly, Eq. (3) gives an area-averaged estimate for the bulk temperature $\langle T_m \rangle$.

Since the boundary conditions at the domain boundaries are in terms of θ , it would appear to be easier to rewrite Eq. 5 in terms of θ and solve directly for θ . However, the evolution equation for θ contains additional terms that represent the evolution of the bulk temperature T_m . Therefore, in order to solve for θ we need to solve an additional equation for T_m . Moreover, solving for the evolution equation for T_m requires the computation of heat flux from every particle that intersects the plane perpendicular to the mean flow at each x location in the direction of the mean flow. Since there is a finite number of particles in the computational domain, the solution may suffer from statistical error. Therefore, it turns out to be easier to transform the periodic boundary conditions on θ to obtain similarity conditions on the temperature field $T(\mathbf{x}, t)$ and solve Eq. (5) for $T(\mathbf{x}, t)$.

In order to simplify the thermal similarity conditions and also to homogenize the boundary conditions on the particle surfaces we define a non dimensional temperature field $\phi(\mathbf{x}, t)$ as follows:

$$\phi(\mathbf{x}, t) = \frac{T(\mathbf{x}, t) - T_s}{T_{m,\text{in}} - T_s} \quad (6)$$

where, $T_{m,\text{in}}$ is the bulk temperature at $x = 0$. Using this definition of the non dimensional temperature, it is easy to see that the non dimensional bulk temperature $\phi_m(x)$ has a similar definition:

$$\phi_m(x, t) = \frac{T_m(x, t) - T_s}{T_{m,\text{in}} - T_s}. \quad (7)$$

Substituting Eq. (6) in Eq. (5) gives the governing equation for the non dimensional temperature:

$$\frac{\partial \phi}{\partial t} + \frac{\partial(u_j \phi)}{\partial x_j} = \alpha_f \frac{\partial^2 \phi}{\partial x_j \partial x_j}. \quad (8)$$

The isothermal boundary conditions on the particle surface reduce to $\phi = 0$.

In order to understand the periodicity conditions and also for ease of implementation we introduce a quantity called the heat ratio r_h which is defined as:

$$r_h = \frac{T_{m,\text{in}} - T_s}{T_{m,\text{out}} - T_s}, \quad (9)$$

where $T_{m,\text{out}}$ is the bulk temperature at $x = L$ and L is the length of the box. The heat ratio is the ratio of the bulk temperature at the inlet ($x = 0$) to the bulk temperature at the outlet ($x = L$). In other words the heat ratio is simply the inverse of the non dimensional bulk temperature at $x = L$ i.e.,

$$r_h = \frac{1}{\phi_{m,\text{out}}}. \quad (10)$$

The heat ratio quantifies by how much a *fluid* particle heats up when it leaves the box and so this quantity depends solely on the flow structure and the interphase heat transfer in the domain. A control volume analysis of the governing equation for ϕ reveals the following relation for the heat ratio:

$$r_h = \frac{T_m(x) - T_s}{T_m(x + L) - T_s} = \frac{T_m(x \pm a) - T_s}{T_m(x + L \pm a) - T_s}, \quad (11)$$

where a is any displacement in the streamwise direction. The periodic boundary conditions on ϕ now appear in a very simple form:

$$\begin{aligned} \phi(0, y, z) &= r_h \phi(L, y, z), \\ \phi(x, 0, z) &= \phi(x, L, z), \\ \phi(x, y, 0) &= \phi(x, y, L). \end{aligned} \quad (12)$$

An important point to be noted is that the heat ratio, or the amount by which the fluid gets heated up (or cooled down) when it reaches the end of the box,

is an unknown quantity and it is part of the solution. In this formulation the thermal similarity conditions (cf. Eq. (12)) are defined in terms of the heat ratio. So the heat transfer problem has to be solved iteratively until the heat ratio converges. In the next section we describe the immersed boundary methodology that is used to solve the heat transfer problem in statistically homogeneous suspensions.

5. Solution Approach

The complete details of the hydrodynamic PReIBM solver are discussed elsewhere (Garg et al., 2010b; Tenneti et al., 2011). Here the discussion is limited to the solution of the heat transfer problem in statistically homogeneous suspensions using PReIBM. In PReIBM, we employ Cartesian grids and solve the mass and momentum conservation equations at all the grid points (including those lying inside the particles). Similarly the nondimensional temperature field is also solved at all grid points. The governing equation for ϕ that is solved in PReIBM is

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u_j \phi)}{\partial x_j} = \frac{\partial q_j^\phi}{\partial x_j} + I_s f_\phi, \quad (13)$$

where $\mathbf{q}^\phi = \alpha_f \nabla \phi$ is the heat flux, and f_ϕ is the additional immersed boundary (IB) forcing term that is nonzero only in the solid phase. The immersed boundary forcing f_ϕ accounts for the presence of the solid particles in the domain by ensuring that the isothermal boundary condition $\phi = 0$ is satisfied on the surface of the solid particles.

The surface of the solid particle is represented by a discrete number of points called boundary points. For spherical particles, the boundary points

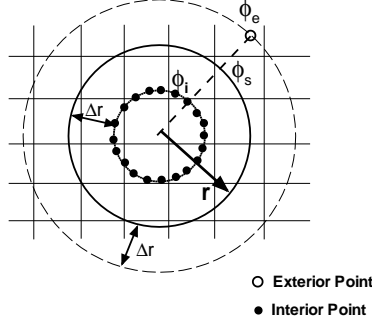


Figure 3: A schematic showing the computation of the immersed boundary forcing f_ϕ for an isothermal particle. The solid circle represents the surface of the particle at r . Open dot shows the location of one exterior point at $r + \Delta r$ (only one exterior point is shown for clarity, although there is one exterior point for each interior point) and filled dots show the location of interior points at $r - \Delta r$ where the immersed boundary forcing is computed. In the schematic, ϕ_e represents the temperature at the exterior point, ϕ_s is the surface temperature while ϕ_i is the temperature at the interior point.

are specified by discretizing the sphere in spherical coordinates. In figure 3, a schematic describing the computation of the IB forcing is shown for the equatorial plane passing through the spherical particle. Another set of points called exterior points are generated by projecting these boundary points onto a sphere of radius $r + \Delta r$, where r is the radius of the particle (see exterior point represented by an open circle on the dashed line in figure 3). Similarly, the boundary points are projected onto a smaller sphere of radius $r - \Delta r$ and these points are called interior points. In our simulations Δr is taken to be same as the grid spacing. The IB forcing is computed only at the interior

points. At these points the fluid temperature is forced in a manner similar to the ghost cell approach used in standard finite-difference/finite-volume based methods (Patankar, 1980). For the boundary condition $\phi = 0$ used in this work, the value of ϕ at the interior points is forced to be opposite in magnitude to the value of ϕ at the corresponding exterior points.

The distinctive feature of PReIBM is that the forcing f_ϕ is computed only at points lying inside the solid particles. This ensures that the fluid-phase temperature field is not contaminated by the scalar IB forcing term f_ϕ , just as the fluid-phase velocity field is not contaminated by the hydrodynamic IB forcing. The consequences of fluid velocity contamination by IB forcing are discussed in detail by Tenneti et al. (2011). The computation of f_ϕ is similar to the computation of the IB forcing for the velocity field. The IB forcing term f_ϕ^{n+1} at the $(n + 1)^{\text{th}}$ time-step is specified to cancel the remaining terms in the governing equation for ϕ and force the nondimensional temperature to its desired value ϕ^d at the interior points:

$$f_\phi^{n+1} = \frac{\phi^d - \phi^n}{\Delta t} + C_\phi^n - \left(\frac{\partial q_j^\phi}{\partial x_j} \right)^n \quad (14)$$

where C_ϕ^n is the convective term at the n^{th} time step.

The heat transfer equation (cf. Eq. 13) in PReIBM is solved using a pseudo-spectral method, with a Crank–Nicolson scheme for the viscous terms, and an Adams–Bashforth scheme for the convective terms. The use of Fourier transforms in the cross stream directions and the Crank–Nicolson scheme in the streamwise direction results in an independent set of cyclic tridiagonal systems that are solved using the Sherman–Morrison formula (Sherman and Morrison, 1950). The coefficient matrices in the tridiagonal systems

depend on the heat ratio r_h which is not known *a priori*. The temperature field is initialized with $r_h = 1$ and the simulation is performed iteratively till the value of the heat ratio converges. It must be noted that in this work we use the steady velocity field that is obtained from the hydrodynamic solver and the velocity field is not advanced during the solution of the heat transfer problem.

6. Results and Discussion

The hydrodynamic solver in the PReIBM methodology has been extensively validated using a comprehensive suite of test cases (Tenneti et al., 2011). In order to check the accuracy of the IB methodology for temperature and also to verify the thermal similarity boundary condition, we simulate convective heat transfer in a square duct. The no slip walls of the duct for the velocity field as well as the isothermal condition at the walls for the temperature field are generated using the IB methodology described in the previous section.

Using an analytical calculation, Shah and London (1978) found that the Nusselt number for a thermally fully developed laminar flow in a square duct is 2.976. We compare the Nusselt number obtained from PReIBM simulations for three different Reynolds numbers with the analytical solution in table 1. We see that the results obtained from PReIBM simulations agree very well with the analytical solution. The numerical convergence of Nusselt number with grid resolution for a Reynolds number of 100 is shown in Figure 4(a). In this figure we plot the relative error between the analytical and numerical solution. We see that the Nusselt number obtained from

Reynolds number	PUReIBM	Analytical
20	3.013	2.976
50	3.029	2.976
100	3.033	2.976

Table 1: Comparison of Nusselt number obtained from PUReIBM simulation of duct flow for three different Reynolds numbers with the Nusselt number derived from an analytical calculation.

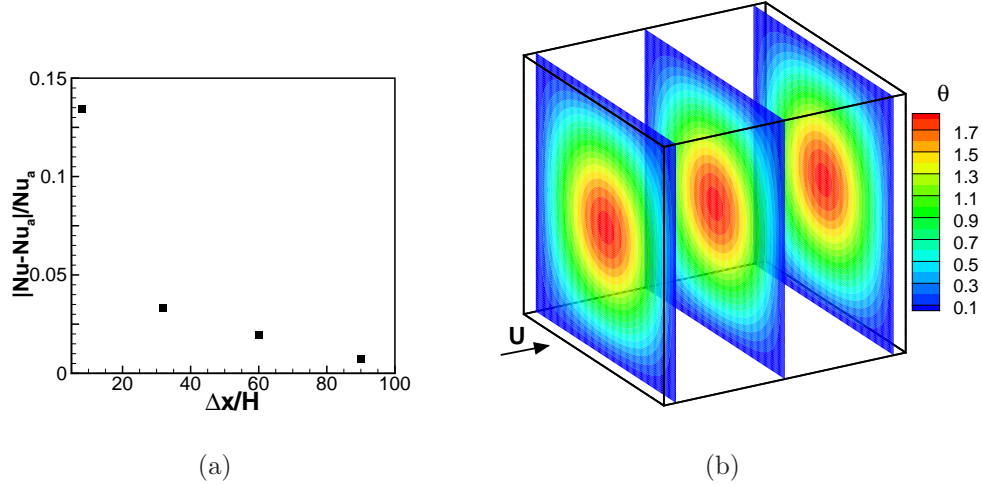


Figure 4: (a) Convergence characteristics of Nusselt number with grid resolution for internal duct flow at a Reynolds number of 100 are shown in. In this plot Nu_a refers to the analytical value of the Nusselt number obtained by Shah and London (1978), Δx is the size of the grid cell and H is the channel height. (b) Contours of the scaled temperature θ are shown in three planes along the direction of the flow shown by the arrow.

PURelBM simulations converge to the analytical value given by Shah and London (1978). In figure 4(b) we plot the contours of the scaled temperature θ (cf. Eq. 4) along the flow direction. This plot verifies that the thermal similarity condition applied at the ends of the domain generates a thermally fully developed flow. These tests confirm the accuracy and numerical convergence of the PURelBM temperature solver and also the correctness of the application of the thermal similarity condition.

We now study heat transfer in statistically homogeneous gas–solid flow using PURelBM DNS of steady flow and heat transfer past stationary, isothermal particles in periodic domains. Particle centers are initialized corresponding to a specified mean solid volume fraction ε_s . The particles are fixed in a random equilibrium configuration they attain following elastic collisions (in the absence of ambient fluid) starting from a lattice arrangement with a Maxwellian velocity distribution. The elastic collisions are simulated using a soft–sphere discrete element model (Cundall and Strack, 1979; Garg et al., 2010a). The pair correlation function at equilibrium specifies the particle configuration for random assemblies. Steady flow is established in the fixed bed by imposing a mean pressure gradient that corresponds to a mean flow Reynolds number. The hydrodynamic solver has been extensively validated in a comprehensive suite of tests (Tenneti et al., 2011). The steady velocity field that is established in the fixed bed is used to evolve the temperature in pseudo–time until the heat ratio reaches a steady state.

The heat transfer problem is statistically inhomogeneous only in the direction of the mean flow and hence all statistics are estimated using area averages in planes perpendicular to the mean flow. Each random particle

configuration is termed a realization of the gas–solid flow corresponding to a specified volume fraction and pair correlation function. The streamwise variation of Nusselt number for the ω^{th} realization is defined as

$$Nu(x; \omega) = \frac{q''(x; \omega) D}{k_f P (\phi_m(x) - \phi_s)}. \quad (15)$$

In this definition, $q''(x; \omega)$ is the interphase heat flux from the particles to the fluid that is averaged in the cross plane at the location x , and P is the perimeter formed by cutting the particles with the plane. The streamwise variation of Nusselt number obtained from a single realization is prone to statistical uncertainty due to finite number of particles in the computational domain. Therefore, the streamwise variation of Nusselt number from a single realization must be averaged over multiple independent simulations (MIS), each corresponding to a different realization of the particle configuration, to get a better estimate for the ensemble–averaged streamwise Nusselt number. If the streamwise Nusselt number obtained from averaging over several realizations is independent of the spatial location, we can say that the Nusselt number is statistically homogeneous. In that case volume averaging can also be used to improve this estimate.

From the PReIBM heat transfer simulations we verify that the thermal similarity boundary condition produces a statistically homogeneous streamwise Nusselt number. Figure 5 shows the streamwise variation of Nusselt number (top panels) for a fixed bed with a solid volume fraction of 0.4 and mean flow Reynolds number of 100. In Fig. 5 we compare the local Nusselt number obtained from averaging over 50 MIS (figure 5(a)) with that obtained from averaging over 5 independent realizations (figure 5(b)). We see that the Nusselt number obtained from 50 MIS is constant along the

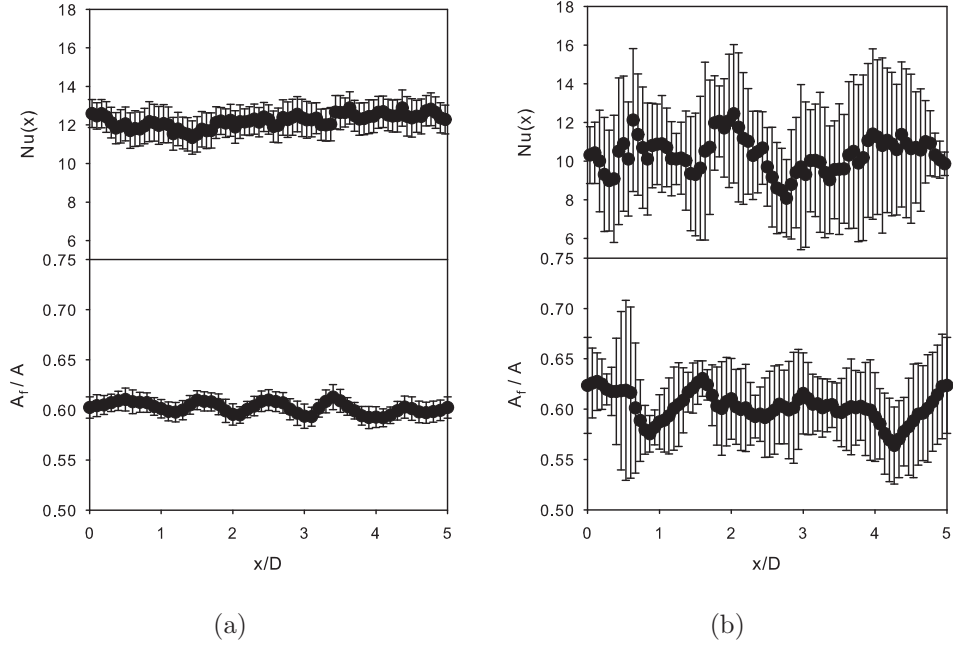


Figure 5: Variation of Nusselt number and the area occupied by the fluid-phase along the direction of the mean flow, obtained from PReIBM simulations of heat transfer in a fixed bed at a volume fraction of 0.4 and mean flow Reynolds number of 100. The local Nusselt number is reported by averaging over (a) 50 and (b) 5 MIS.

flow direction. The Nusselt number from 5 MIS shows some variation along the axial direction. The finite size of the computational domain in the cross stream direction and also the small number of independent realizations are responsible for this streamwise variation in the Nusselt number. To see this more clearly, the variation of the area occupied by the fluid A_f along the flow direction is also shown in Fig. 5 (bottom panels). Recall that one of the conditions for statistical homogeneity of Nusselt number is that the area occupied by the fluid should be constant along the flow direction. The figures indicate that the estimate for the average area occupied by the fluid can vary along the flow direction and also at any given axial location there are fluctuations in the area across realizations (indicated by error bars). The amplitude of the fluctuation in the area is found to be about 7% when the averaging is performed over 5 MIS. From convergence studies, we found that 50 realizations are required to reduce the amplitude in the fluctuation of the area to 2%. Similar requirements on the number of independent realizations were reported by Xu and Subramaniam (2010) in their study of particles in upstream turbulence. Figure 5(a) shows that the variation as well as the level of fluctuations in the Nusselt number and the area fraction are reduced when the averaging is performed over 50 MIS. We conclude that for statistically homogeneous assemblies, the formulation developed for the heat transfer problem ensures that the local Nusselt number is statistically homogeneous.

Due to the statistical homogeneity of the Nusselt number in the stream-wise direction, we can compute the average Nusselt number $\langle \text{Nu} \rangle$ by averaging $Nu(x)$ along the axial direction. Figure 6 shows compares the average

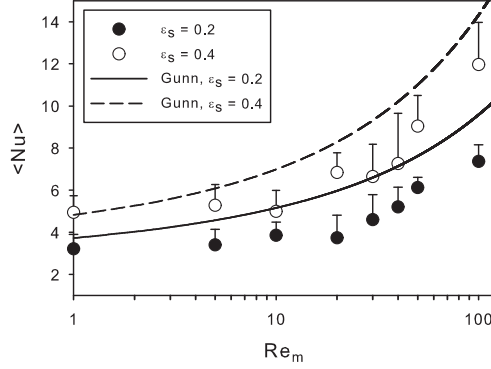


Figure 6: Behavior of the average Nusselt number $\langle \text{Nu} \rangle$ with mean flow Reynolds number for two solid volume fractions. Symbols indicate data obtained from PReIBM simulations while the solid lines are obtained from Gunn's correlation (Gunn, 1978).

Nusselt number obtained from PReIBM simulations with the Nusselt number predicted by Gunn's correlation (Gunn, 1978). From the figure we see that the average Nusselt number increases with both solid volume fraction and mean flow Reynolds number and this behavior is consistent with the trend predicted by the correlation. It must be noted that the Nusselt number correlation given by Gunn (1978) is a fit to experimental data obtained by several researchers for packed beds ($\varepsilon_s = 0.6$). Given that the experimental data itself has a wide variation, the agreement between the PReIBM DNS and the correlation is excellent.

In addition to the average Nusselt number, the nature of inhomogeneity of the fluid temperature field or fluid heating is important in modeling the average interphase heat transfer $\langle Q_{g-s} \rangle$. We plot the non-dimensional bulk temperature ϕ_m along the flow direction for two mean flow Reynolds numbers (1 and 100) and two solid volume fractions (0.2 and 0.4) in figure 7(a).

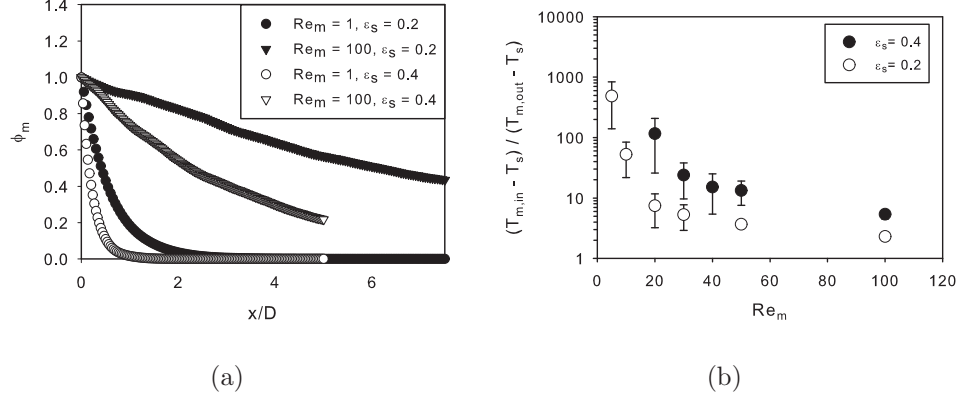


Figure 7: (a) Variation of the nondimensional bulk fluid temperature along the axial direction for two mean flow Reynolds numbers (1 and 100) and two solid volume fractions (0.2 and 0.4). (b) Behavior of heat ratio with Reynolds number for two solid volume fractions (0.2 and 0.4).

The results confirm the fact that the temperature field is not homogeneous in the flow direction. We see that the fluid heating (or cooling) is high particularly for high solid volume fraction and low Reynolds number. This result is more easily evident when we consider the behavior of heat ratio r_h . Recall that the heat ratio gives a measure of the fluid heating or cooling. Figure 7(b) shows that the heat ratio is close to unity only at high mean flow Reynolds numbers. The scale of variation of ϕ_m in Fig. 7(a) indicates that the mean fluid temperature can be inhomogeneous on the scale of a few particle diameters, whereas two-fluid models assume this field is homogeneous on the scale of a grid cell. Therefore, the inhomogeneity of the average fluid-phase temperature cannot be neglected in the CFD implementations of models for average gas-solid heat transfer.

7. Conclusions

In this work we present a particle-resolved direct numerical simulation methodology to study heat transfer in statistically homogeneous gas-solid flow. The Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (Tenneti et al., 2011) (PUReIBM) has been extended to investigate heat transfer in fixed periodic assemblies of monodisperse spherical particles held at a constant uniform temperature. Periodic arrangement of particles induces a velocity field that is periodic in all three directions. Since the mean fluid velocity has a direction and all the particles are held at the same temperature, the resulting temperature field will not be periodic. In order to be consistent with the periodic arrangement of the particles, a thermal similarity boundary condition is applied on the temperature field by drawing analogy from thermally fully developed flow in pipes. The extension of PUReIBM to solve for the temperature field is validated by solving the heat transfer problem in a square duct. Numerical convergence and the validity of the thermal similarity condition in flow past random assemblies of spheres is verified. From PUReIBM PR-DNS of heat transfer in fixed particle assemblies, we establish that the formulation developed for heat transfer results in a statistically homogeneous average Nusselt number. We conclude that fluid heating is important in gas-solid systems of high solid volume fraction and low mean flow Reynolds number. Two-fluid CFD models that are used to solve for heat transfer in gas-solid systems need to account for the inhomogeneity in average temperature fields that is caused by fluid heating.

Appendix A. Regime of applicability of the assumptions

The assumptions employed in this work and their regime of validity are discussed in this section. The use of a fixed bed setup for gas–solid flows is justified if the configuration of the particles changes very slowly compared to the time it takes to attain mean momentum balance. The time scale over which the particle configuration changes depends on $\text{Re}_\Theta = D\Theta^{1/2}/\nu_f$, which is the Reynolds number based on the particle fluctuating velocity that is characterized by the particle granular temperature Θ . The particle granular temperature Θ is a measure of the variance in the particle velocities and is defined as $\Theta = 1/3 \langle \mathbf{v}'' \cdot \mathbf{v}'' \rangle$, where \mathbf{v}'' is the fluctuation in the particle velocity defined with respect to the mean particle velocity. Particle–resolved simulations of freely evolving suspensions (Tenneti et al., 2010) and recent high–speed imaging of particles (Cocco et al., 2010) show that this value of Re_Θ is $\mathcal{O}(1)$ for high Stokes number particles that are characteristic of gas–solid flows (e.g., coal particles in air).

An important simplification made in this work is the use of a uniform temperature for the particles. The extent of variation of the temperature inside a particle is governed by the Biot number (Bi), which is defined as $\text{Bi} = hD/k_s$. In this definition h is the convection heat transfer coefficient between the particle and the fluid, and k_s is the thermal conductivity of the solid. For many gas–solid systems the thermal conductivity of the solid is greater than that of the gas by more than an order of magnitude (e.g. air–coal, air–Ferrous oxide, air–fused silica) and results in a Biot number that is less than 0.1. The small Biot number encountered in many practical gas–solid systems suggests a lumped capacitance model for the particle temperature, where the spatial

variation of temperature inside the particle can be neglected.

In addition to the assumption of uniform temperature of the particle, we also assume that this uniform temperature is constant in time i.e., we assume the particles are isothermal. This simplification follows from the observation that the thermal response time of the particles is large compared to the time it takes for the fluid to travel a distance equal to the particle diameter. The thermal response time of the particle $\tau_{tp} \sim hA_s / (mC_{ps})$, where A_s is the surface area, m is the mass and C_{ps} is the specific heat of the particle, respectively. The time taken by the fluid to travel over a particle $\tau_f \sim D / |\langle \mathbf{W} \rangle|$, where $\langle \mathbf{W} \rangle$ is the mean slip velocity between the particle and the fluid. The ratio of these time scales

$$\frac{\tau_{tp}}{\tau_f} \sim \left(\frac{\rho_p C_{ps}}{\rho_f C_{pf}} \right) \left(\frac{\text{Re}_m \text{Pr}}{\text{Nu}} \right),$$

where ρ_p is the density of the particle, ρ_f is the density of the fluid, C_{pf} is the specific heat of the fluid and Nu is the Nusselt number. Experimental studies (Gunn, 1978) of heat transfer in gas–solid systems reveal that the ratio $\frac{\text{Re}_m \text{Pr}}{\text{Nu}} \sim \text{O}(1)$. For gas–solid flows the ratio of the density of the particles to the density of the fluid density is very high ($\sim \text{O}(10^3)$). Due to the high thermal inertia of the particles the thermal response time of the particles is about three orders of magnitude larger than the convective time scale of the fluid. Hence, the uniform temperature of a particle can be assumed to be constant in time. In addition to the assumption of a uniform and constant particle temperature, we also assume that all particles in the bed are maintained at the same temperature. The assumption that the particles equilibrate to the same surface temperature is consistent with earlier works (Gunn, 1978; Acrivos et al., 1980).

Neglecting viscous dissipation, radiation and free convection effects limits the gas–solid systems to which our simulation methodology applies. Viscous heating becomes important in flows with Mach numbers comparable or greater than unity and since we are concerned with subsonic flows, viscous dissipation is neglected in this work. Free convection is quantified by the Grashof number, which is defined as

$$\text{Gr} = \frac{g\beta(T_f - T_s)D^3}{\nu_f^2}, \quad (\text{A.1})$$

where T_f is the free stream temperature, T_s is the temperature of the solid surface, and β is the volumetric thermal expansion coefficient ($\beta = 1/T_f$ for gases). Free convection effects can be neglected if $\text{Gr}/\text{Re}_m^2 < 1$. For each Reynolds number, this constraint imposes an upper limit on the particle diameter above which free convection effects cannot be neglected. For a given value of T_f/T_s , the upper limit on the particle diameter D increases with increasing Reynolds number. If a typical value of 100 is taken for the fluid to solid temperature ratio (i.e. $T_f/T_s = 100$), and air is assumed to be the fluid under terrestrial conditions ($g = 9.81 \text{ m/s}^2$), then for a Reynolds number $\text{Re}_m = 1$ the particle diameter has to be less than $350 \mu\text{m}$ for negligible free convection. This restriction on the particle diameter becomes less severe as the Reynolds number increases.

For an isolated particle at T_s with emissivity equal to one, and surrounded by fluid at T_f , the ratio of radiation to forced convection heat transfer can be expressed as

$$\hat{q}_{\text{rc}} = \frac{q_{\text{rad}}}{q_{\text{conv}}} = \frac{\sigma(T_s + T_f)(T_s^2 + T_f^2)}{h_{\text{fs}}} = \frac{\sigma D(T_s + T_f)(T_s^2 + T_f^2)}{\text{Nu } k_f},$$

where $\sigma = 5.67 \times 10^{-8} \text{ W/m}^2\cdot\text{K}^4$ is the Stefan–Boltzmann constant. Assuming air to be the surrounding fluid at $T_f = 1000\text{K}$ ($k_f = 0.060 \text{ W/m}\cdot\text{K}$) and the particle temperature $T_s = 300\text{K}$, for Stokes flow (i.e. $\text{Nu} \approx 2$) the ratio of radiation to forced convection heat transfer increases linearly with particle diameter from 0.66×10^{-4} to 0.66×10^{-2} , for particle diameter in the range 1 to 100 microns. While this estimate is valid in the Stokes flow regime, with increasing Reynolds number the higher value of average Nusselt number reduces the ratio of radiation to forced convection heat transfer, thus relaxing the restriction on particle diameter. These estimates of the relative importance of forced convection to free convection and radiation heat transfer show that the restriction on particle diameter is most severe in the Stokes flow regime, and is progressively less restrictive with increasing Reynolds number. Therefore, the assumptions used in this work are indeed applicable and relevant to practical gas–solid systems.

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