Intra- and Inter-Particle Resolved Simulations and Experiments on Thermal Transport in Confined Particle Beds

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Introduction

Models for thermal transport in dense fluid-particle suspension flows often rely on a number of assumptions, e.g., (i) a uniform intra-particle temperature profile, or (ii) a two dimensional formulation of the flow system. We established a generic, three-dimensional open-source simulation environment [1,2] to help in relaxing some of these assumptions. Our new simulation environment allows one (i) to derive closures for per-particle heat transfer, as well as (ii) to consider intra-particle temperature profiles in Euler-Lagrange simulations (see Fig. 1). Here we demonstrate the fidelity of our tools using a set of benchmark simulations involving canonical flow situations.

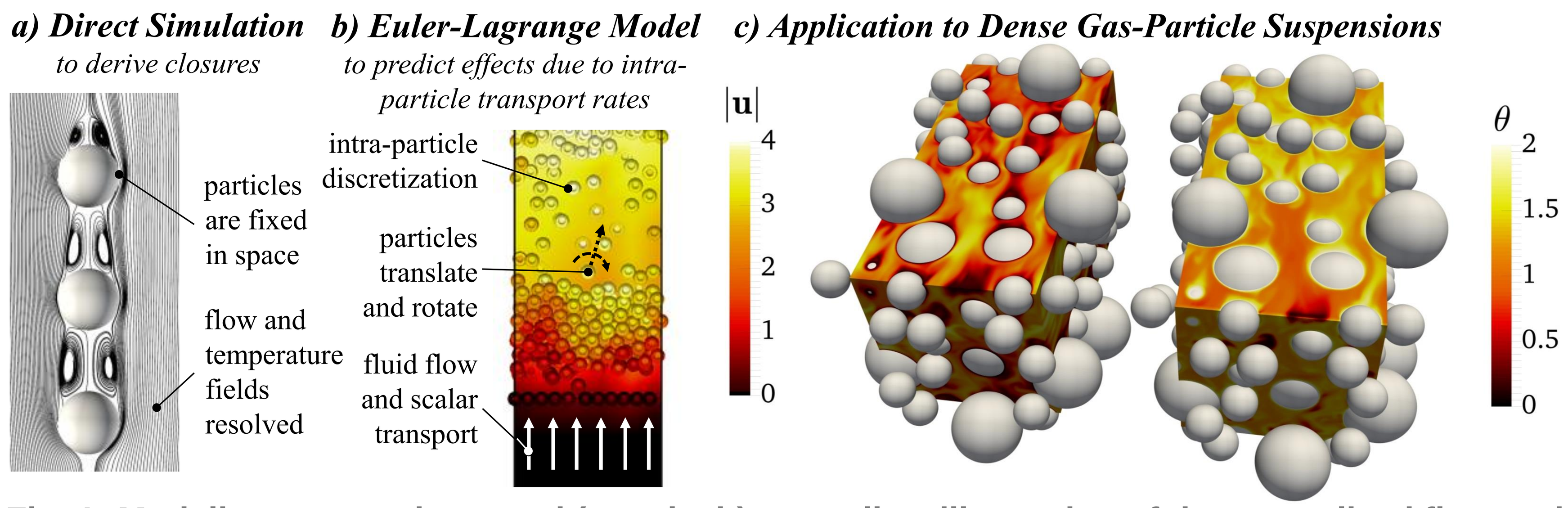

Fig. 1: Modeling approaches used (panel a,b), as well as illustration of the normalized flow and temperature field in a dense bi-disperse gas-particle suspension (panel c).

A Novel Hybrid FD/IB Method

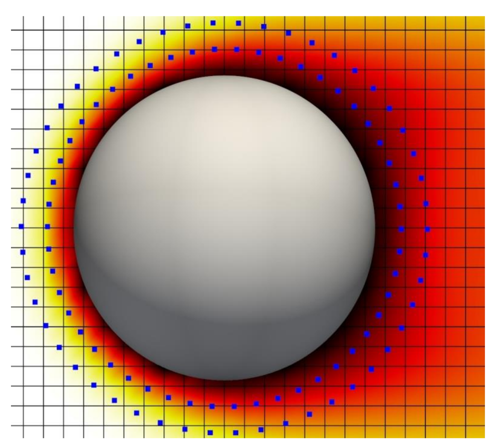

Fig. 2: Illustration of the HFD-IB algorithm.

We use Direct Numerical Simulations (DNS) relying on a novel Hybrid Fictitious Domain / Immersed Boundary algorithm (HFD-IB, [3]). This algorithm imposes rigidity inside the immersed bodies, and applies a Dirichlet boundary condition at the immersed surfaces using a second order accurate method. Specifically, we rely on a reconstruction of the flow and concentration field in the vicinity of the immersed surface using an interpolation technique (see blue dots in Fig. 2).

Per-Particle Transfer Coefficients

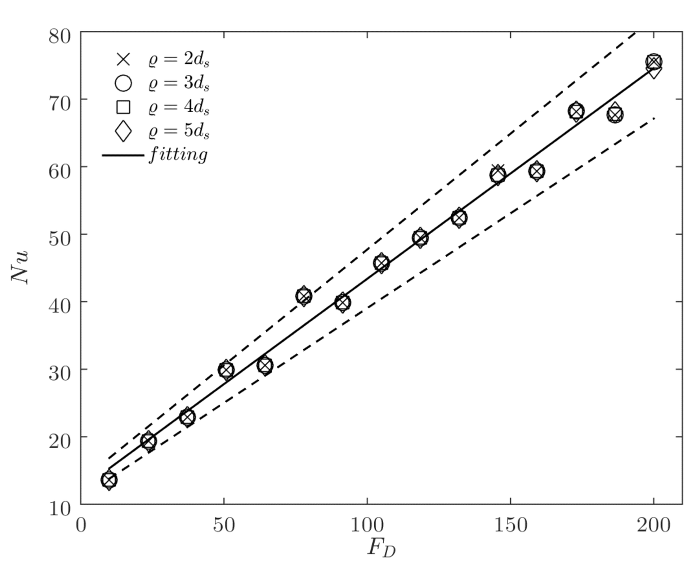

Fig. 3: Correlation between normalized drag force and particle-based Nusselt number in a bi-disperse suspension.

Currently, available closures attempt to model *average* transfer rates of momentum, heat, or species from a particle assembly. This is in contrast to the need for a *per-particle* transfer model to be used in Euler-Lagrange models.

We make use of the filtering toolbox "CPPPO" [4] to draw relevant statistics from a set of DNSs considering dense bi-disperse particle clouds. We then establish a model for predicting per-particle drag coefficient based on a Maxwell-Boltzmann distribution. Additionally, we asses the existence of an analogy between drag coefficient and per-particle Nusselt number (see Fig. 3).

Euler-Lagrange Model & Intra-Particle Effects

Our Euler-Lagrange model relies on the tools CFDEM® and LIGGGHTS®, and does not resolve flow details around the particle. Instead, we model the effect of the surrounding fluid based on the previously developed closures. Intra-particle temperature profiles are predicted by using the tool "ParScale" [1], which approximates Eqn. (1) using spherical symmetry. Eqn. (1) is subject to a fixed gradient boundary conditions set by a predefined heat transfer rate.

$$\partial_t T + \nabla \cdot (-\lambda \nabla T) = 0 \quad (1)$$

Thermal Transport in the Bulk

We next aim on quantifying the effect of intra-particle heat conduction on thermal transport rates in a sheared granular material by:

- **Enforcing a Lees-Edwards shear flow, as well as a fixed temperature gradient to the bed of mono-disperse particles.**
- **Modelling heat exchange with the surrounding fluid phase using a constant heat transfer coefficient.**

We find that:

- **Intra-particle temperature gradients are relevant for moderate *Bi* , i.e., for *Bi* > 10^{-2}.**
- **Convective thermal transport exceeds conduction even at moderate granular *Pe* (i.e., *Pe* > 0.01).**

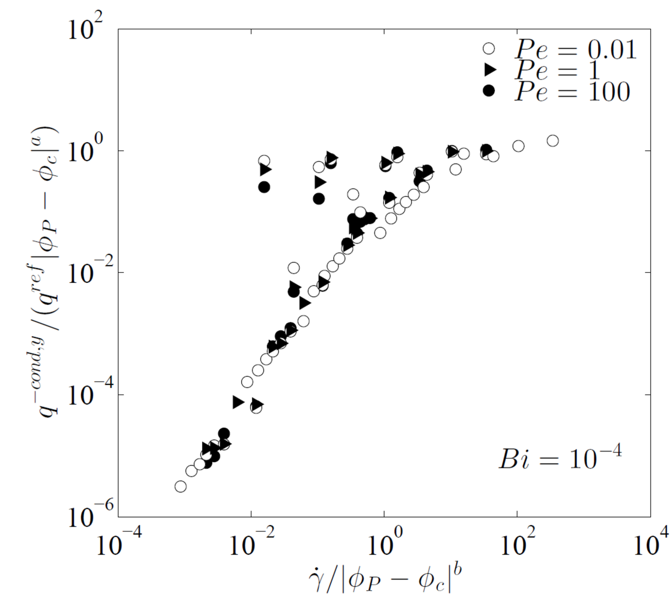

Fig. 4: Influence of the Pelect number on the conductive heat flux in different regimes of granular flow (slow cooling characterized by *Bi* = 10^{-4}).

Heat Transfer in Wall Bounded Domains

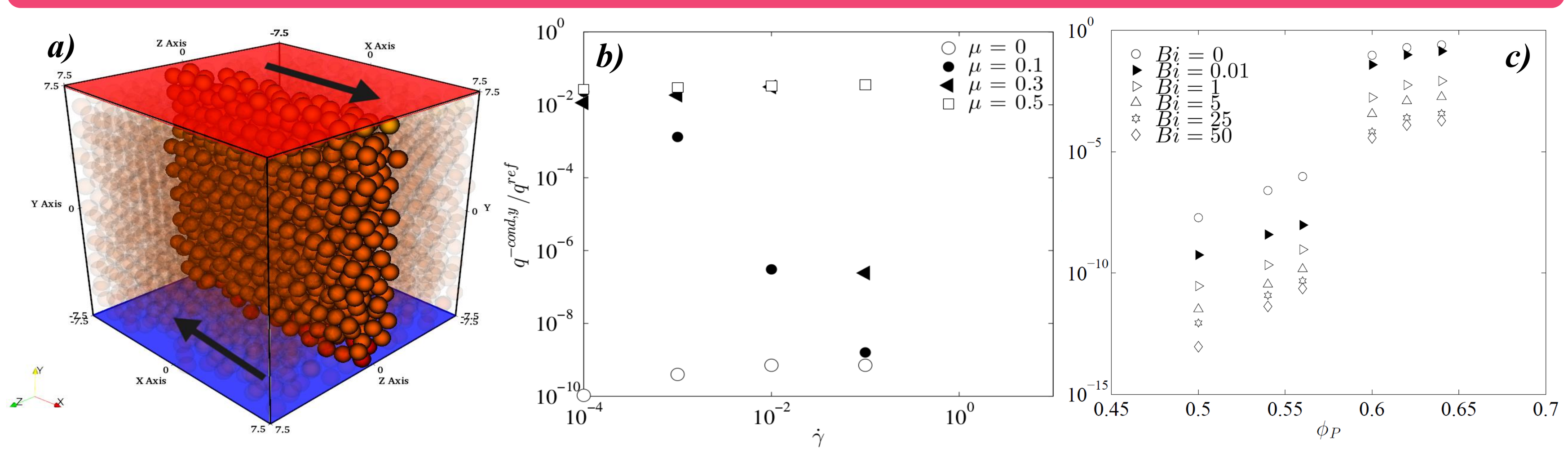

Fig. 5: Simulation setup for wall bounded shear flow simulation with constant wall temperatures (panel a). Conductive heat flux for crystallized and non-crystallized granular materials (panel b, *Pe* = 0.01, *Bi* = 0.1 and φ_p = 0.64). Effect of jamming (panel c, *Pe* = 0.01).

To complete our model for predicting thermal transport rates in granular materials, we next study granular flow between infinitly long walls moving in counter-wise direction [5]. Wall temperatures are kept constant to impose a temperature gradient. We find that the heat conduction flux experiences (i) a large drop in case of crystallization (i.e., ordering of particles, panel b) and (ii) a jump in case of jammed states (panel c). Surprisingly, the granular convective heat flux is unchanged when crossing the critical jamming particle volume fraction.

Analytical Model & Experiments

We benchmark our simulation tools against a number of analytical solutions, e.g., that of Schumann [6]. Also, we employ a semi-analytical solution to a 1D model (shown in Eqn. 2) for the mean particle temperature considering the dispersion due to random particle motion.

$$\partial_t T_p = 6\alpha / \left(d_p \rho_p c_{P,p}\right)\left(T_f - T_p\right) + D_p \partial_{zz} T_p \quad (2)$$

Fig. 6 illustrates the outcome of some of these benchmark simulations, verifying our implementation, and highlighting some Biot-number effects. Also, a benchmark against experimental data is presented.

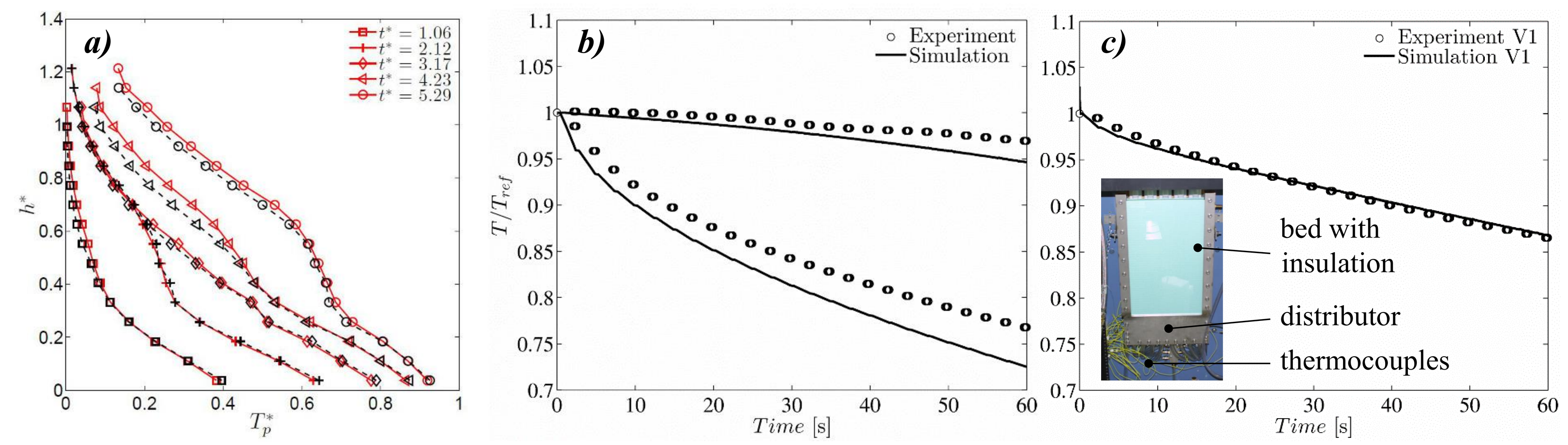

Fig. 6: Temporal progression of the mean particle temperature vs. bed height in a fluidized bed based on CFD-DEM simulations with ParScale (panel a, solid lines, *Bi* = 0.8), and using a semi-analytical solution to Eqn. 2 (dashed lines). Horizontal mean fluid temperatures at different positions in a fixed bed consisting of high-Biot number particles (panel b,c).

Conclusion & Outlook

Our newly developed closures account for the per-particle variability of transfer coefficients for momentum and energy. Our simulation platform can account for intra particle temperature profiles. We show that these effects should be considered, even at moderate Biot numbers, i.e., *Bi* > 10^{-2}, and slowly-sheared flows.

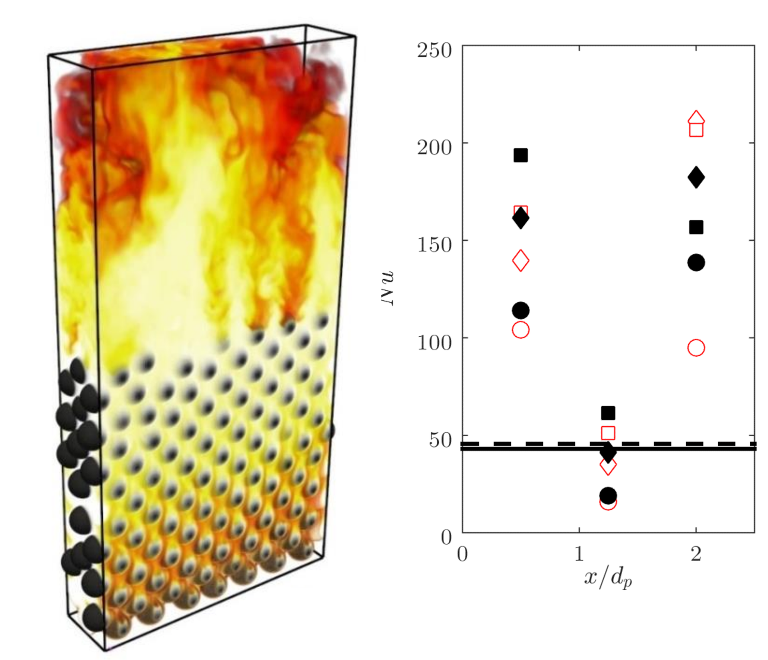

Fig. 7: Wall effect quantified via DNS of heat transfer from a particle bed (*x* is the wall-normal distance; symbols represent different axial positions and filter sizes).

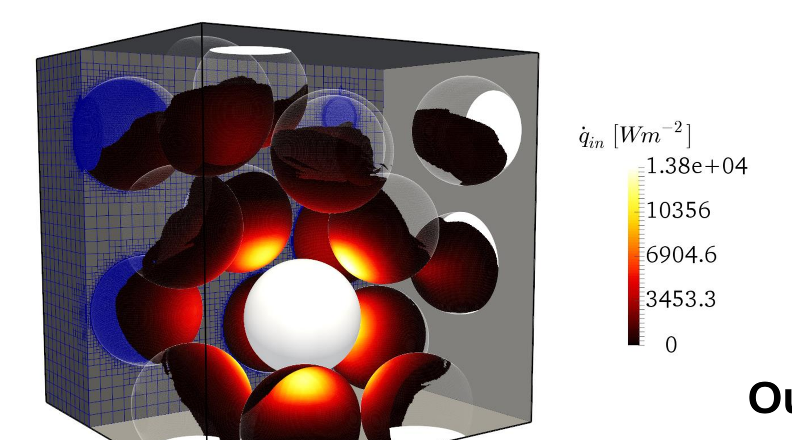

Fig. 8: Distribution of the incident radiative heat flux predicted by a finite-volume/discrete-ordinate method.

Our current efforts aim on expanding the applicability of our tools to account for (i) wall effects (see Fig. 7), as well as (ii) more extreme temperature gradients for which radiation becomes the leading thermal transfer mechanism (see Fig. 8).

Nomenclature

Bi	Biot number	*i*	particle index	*t*	time	μ	friction coefficient
d_p	particle diameter	*Nu*	Nusselt number	*T*	Temperature	θ	normalized temperature
F	drag coefficient	*q*	heat flux	*u*	velocity	ρ	normalized filter size
*h**	dimensionless height	*Pe*	Peclet number	ϕ_p	particle volume fraction		

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