Particle - Resolved Simulation of Anisothermal Fluidized Beds

Edouard Butaye¹, Rémy Quintana¹, Adrien Toutant¹, Samuel Mer¹, Françoise Bataille¹

¹Laboratory PROMES-CNRS (UPR 8521), Univ. Perpignan Via Domitia Perpignan, France edouard.butaye@promes.cnrs.fr; adrien.toutant@univ-perp.fr

Abstract – Fluidized beds are used as a new heat transfer fluid in solar tower power plants. To optimize heat transfer in solar receivers, it is essential to characterize the heat exchange between the walls and the particles. Particle – Resolved Direct Numerical Simulation (PR-DNS) is thus used to study hydrodynamic interactions and heat flux in an anisothermal fluid – solid particles assembly. An original method was developed to compute hydrodynamic forces and thermal flux over the surface of the solid particle. In PR-DNS, velocity gradients and pressure are fully resolved in the vicinity of the interfaces between the fluid and the particles. However, PR-DNS requires several dozen of meshes in the particle's diameter and is therefore not suitable for the simulation of fluidized beds. To overcome this issue, Particle-Resolved Subgrid Corrected Simulation (PR-SCS) is introduced. In this framework, a coarse mesh is employed, and the partially captured velocity gradients and pressure are corrected by means of a mesh-dependent numerical correction. The method is validated for a single particle settling in an infinite medium, and then adapted to fluidized beds. The same methodology is developed for anisothermal flows. The heat flux received by the particle is computed over its surface. The numerical error due to mesh coarseness is corrected with a mesh-dependent correction. Finally, the collective effects of particles are examined in an anisothermal fluidized bed.

Keywords: Particle - Resolved Simulation, fluidized bed, DEM, hydrodynamic force computation, anisothermal flow

1. Introduction

Fluid particle flows are widely employed in the industry for catalytic reactions, pneumatic transport, crystallization processes or power generation in solar towers power plants. In the context of solar power generation, fluidized beds are used as a new heat transfer fluid within vertical tubular receivers in solar towers power plants. Indeed, actual heat transfer fluids – such as molten salt or oils – are limited to 800K due to thermodynamic considerations. To overcome this issue and reach a higher temperature, the use of solid particles is considered. While homogeneously blowing an air flow below a particle bed, above a threshold velocity, fluid properties are attributed to the air -solid mixture (mixing viscosity, bubby flow, waves...). Over the last decades, experimental studies have described fluidized beds behavior [1-2]. To optimize heat transfers between the particles and the walls of the solar receiver, a local description of interactions between the fluid, the particles, and the walls, is required. However, experimental characterization of the flow inside solar receivers remains difficult without invasive methods. Numerical study is therefore essential to fully characterize the flow.

Numerous methods and resolution scales are available in the literature to study fluid – particles flows [3-5]. To compute the hydrodynamic forces exerted by the fluid on the particle surface, Particle-Resolved Simulations (PRS) constitute an excellent tool. To fully resolve the velocity gradients and the pressure at the interface between the two media, several dozen meshes per particle's diameter are required. In Stokes configuration, for which convective effects are negligible compared with diffusive effects, 40 meshes per diameter are required to solve hydrodynamic gradients at the interface. The higher the Reynolds number, the thinner the dynamic boundary layer and the higher the grid resolution required to fully resolve the gradients. Simulations with fully resolved gradients are referred to as Particle-Resolved Direct Numerical Simulation (PR-DNS). The computational cost associated with PR-DNS limits its application to academic cases. For this reason, many Particle-Resolved Simulations of fluidized beds are computed with only a dozen meshes in the particle's diameter, typically between 10 and 16 [6-8]. In these cases, velocity gradients and pressure are not accurately calculated at the interface, leading to an error in the hydrodynamic forces exerted by the fluid on the particle's interface and thus to the particle's velocity. To overcome this issue, we propose to consider Particle-Resolved Sub-grid Corrected Simulations (PR-SCS). The same grid resolution is used for both PRS and PR-SCS, but a numerical correction on the hydrodynamic forces is applied to each particle in PR-SCS to correct the unresolved part of the friction. This method is presented and validated in

[9] for a single particle in sedimentation in an infinite medium and is now assessed in the context of a liquid-solid fluidized bed. A similar methodology is applied to correct sub-resolution effects on the particle heat flux calculation.

The modeling approach is presented in section 2 and PR-SCS for a single particle in sedimentation is assessed in section 3. Finally, a liquid-solid anisothermal fluidized bed is investigated in section 4.

2. Modeling

The numerical modeling strategy is based on the one-fluid VOF/Front-Tracking method implemented in TrioCFD software. Initially developed for gas-liquid flows, Hamidi *et al.* have extended the method to fluid-solid particles [8]. Solid behavior of particles is ensured by a viscous penalization and collisions are handled with a DEM approach. The energy equation is solved considering the temperature as a passive scalar. A phase indicator function is integrated over the volume of each cell of the computational domain. It is used to compute fluid properties in two-phase cells. Pressure and velocity fields are discretized over a staggered grid while the interface is located thanks to Lagrangian markers accordingly to the Front-Tracking method (see Fig. 1).

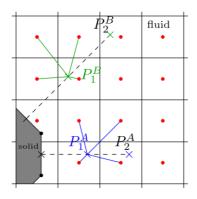


Fig. 1: Identification of neighboring Eulerian meshes for the hydrodynamic force computation. .: pressure and temperature

nodes, .: Lagrangian marker, x, x: interpolation points, x: Lagrangian facet.

Pressure and friction forces are computed on each Lagrangian facet based on the fluid properties. At the interface between the fluid and the solid, the Eulerian cells are, by definition, two-phase. It is therefore required to move away from the interface along the normal to evaluate fluid properties in purely fluid cells. Two points, noted P1 and P2, are identified to compute fluid velocity, pressure and temperature with a trilinear interpolation using neighboring grid cells (see Fig. 1). Then, a linear extrapolation of the pressure in P1 and P2 gives the pressure at the gravity center of the Lagrangian facet. For the velocity and the temperature, a second order forward discretization scheme is employed to compute the velocity and the temperature gradients at the interface. Finally, an integral over the particle surface gives the pressure and friction forces as well as the heat flux received by the particle from the fluid. More details on the numerical method can be found in [9].

3. Validation of the method

The methodology is assessed through the study of Stokes configuration, the theoretical expression of hydrodynamic forces being well known. First, a mesh convergence study is performed to quantify the error committed on the hydrodynamic force computation due to the coarseness of the mesh, noted PRS in Fig.2. Then, a correction is computed for each grid resolution to obtain a zero error in the hydrodynamic force computation, noted Fc in Fig.2. Interpolation of the results of this convergence study leads to the following correction, where x represents the grid resolution:

$$F_c(x) = \frac{9.79}{x^{1.95}} F_{Stokes}$$
(1)

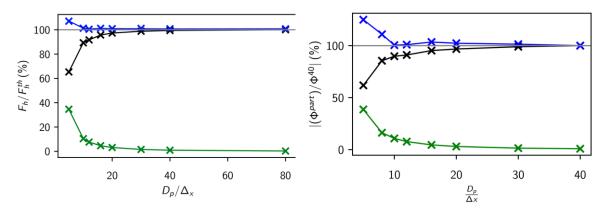


Fig. 2: Overall hydrodynamic force, normalized by its theoretical value, as a function of the mesh resolution (left). Heat flux received by the particle from the fluid, as a function of the mesh resolution (right).

The same methodology is applied to heat flux. However, in this case the theoretical heat flux is not known and the grid resolution of 40 meshes per diameter is considered as the reference. For both hydrodynamic force and heat flux, PR-SCS improve the accuracy of the simulations by 10 % at a grid resolution of 10 meshes per diameter.

4. Fluidized beds

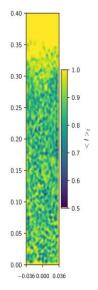


Fig. 3: Time-space average of the integrated phase indicator function (unconverged statistics). The spatial average is computed at the center of the domain, over a thickness of one particle diameter. Fluidization velocity: 0.15m/s

PR-SCS is then assessed on a liquid-solid anisothermal fluidized bed of 2134 particles. The simulation reproduces the experiment of Aguilar-Corona *et al.* [10], numerically reproduced by Ozel *et al.* [6] and Hamidi *et al.* [8]. Two fluidization velocities are investigated, v=0.073 m/s and v=0.15m/s and two grid resolutions – 12 and 24 meshes per particle diameter – are performed for the lowest fluidization velocity. A statistical study is performed for the fluid velocity, phase indicator function and temperature. In addition, hydrodynamic forces and heat transfer flux are post-processed for each particle. Temporal average and RMS of this data inform on the collective effects of a fluid-particle assembly. Work in progress will focus on a detailed analysis of the hydrodynamic forces and heat flux received by each particle of the bed. A statistical study on particles' positions and velocities as well as hydrodynamic properties will also be carried out.

5. Conclusion

The objective of the present paper was to clarify fluid-particle interactions for PRS. A distinction between PR-DNS – with fully resolved gradients at the interface between the fluid and solid particles – and PRS with coarse grid resolution was presented. Hydrodynamic forces exerted by the fluid over the particle's surface and heat flux received by the particle were

computed on a single particle in sedimentation in an infinite medium. A convergence study was conducted to develop a mesh-dependent correction to correct the sub resolution of gradients at the interface on coarse meshes. To assess PR-SCS in more complex flows, an anisothermal fluidized bed was studied for two grid resolutions.

Acknowledgements

This work was granted access to the HPC resources of CINES under the allocation 2022-A0122B11441 made by GENCI. The authors gratefully acknowledge the CEA for the development of the TRUST platform. The technical support of TRUST/TrioCFD team was also greatly appreciated.

References

- [1] R. Boissiere, R. Ansart, D. Gauthier, G. Flamant, M. Hemati, "Experimental study of gas-particle dense suspension upward flow for application as a new heat transfer and storage fluid," Can. J. Chem. Eng., 2014.
- [2] R. Gueguen, G. Sahuquet, S. Mer, A. Toutant, F. Bataille, G. Flamant, "Gas-solid flow in a fluidized-particle tubular solar receiver: Off-sun experimental flow regimes characterization," Energies, vol. 14, 2021.
- [3] F. Alobaid, N. Almohammed, M.M. Farid, J. May, P. Rößger, A. Richter, B. Epple, "Progress in cfd simulations of fluidized beds for chemical and energy process engineering," Progress in Energy and Combustion Science, vol. 91, 2022.
- [4] N.G. Deen, M. Van Sint Annaland, M.A. Van der Hoef, J.A.M. Kuipers, "Review of discrete particle modeling of fluidized beds," Chem. Eng. Sci., vol. 62, 2007.
- [5] M.A. van der Hoef, M. Ye, M. Van Sint Annaland, A.T. Andrews IV, S. Sundaresan, J.A.M. Kuipers, "Multiscale modeling of gas-fluidized beds," Adv. Chem. Eng., vol 31, 2006.
- [6] A. Ozel, J.C. Brändle de Motta, M. Abbas, P. Fede, O. Masbernat, S. Vincent, J.-L. Estivalezes, O. Simonin, "Particle resolved direct numerical simulation of a liquid-solid fluidized bed: Comparison with experimental data," Int. J. Multiph. Flow, vol. 89, 2017.
- [7] Y. Tang, E.A.J.F. Peters, J.A.M. Kuipers, "Direct numerical simulation of dynamic gas-solid suspensions," AIChE J., vol. 62, 2016.
- [8] M.S. Hamidi, A. Toutant, S. Mer, F. Bataille, "Assessment of a coupled VOF-Front-Tracking/DEM method for simulating fluid-particles flows," Int. J. Multiph. Flow, vol. 165, 2023.
- [9] E. Butaye, A. Toutant, S. Mer, F. Bataille, "Development of Particle Resolved Subgrid Corrected Simulation," Submitted to Comput. Fluids.
- [10] A. Aguilar-Corona, R. Zenit, O. Masbernat, "Collisions in a liquid fluidized bed," Int. J. Multiph. Flow, vol. 37, 2011.