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Rising of 3D catalyst particles in a natural convection dominated flow by a parallel DNS method

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ABSTRACT

We investigate the problem of particulate flows with heat transfer by parallel direct numerical simulation (DNS). Among other heat transfer problems, we examine in detail the case of a 3D spherical catalyst rising in an enclosure due to natural convection though it is heavier than the suspending fluid. Natural convection is created by heat transferred from the warmer particle to the fluid. Heat is assumed to be produced at a constant rate in the particle bulk. As expected, there exists a critical production rate that leads to the rising of the catalyst. Compared to the 2D circular cylinder counterpart, momentum and heat transfers are slower in 3D and the spherical catalyst rises for a lower production rate. At the numerical level, we employ a Distributed Lagrange Multiplier/Fictitious Domain formulation together with an operator-splitting algorithm to solve the coupled problem. Two families of Lagrange multiplier are introduced to relax the velocity and temperature constraints respectively. As suggested in Wachs (2009), particle collisions are handled by an efficient Discrete Element Method granular solver. As it is, the model is restricted to the case of homogeneous temperature over the particles. From a computational viewpoint, this work might be regarded as an extension of the method proposed in our previous contributions (Dan & Wachs, 2010; Yu, Shao, et al., 2006) to distributed computing with our new parallel code PeliGRIFF.[1] This opens up new possibilities to study a broad range of applications in 3D and to get more insight in the comprehension of particulate flows with heat transfer. In particular, we examine how a bed of spherical catalysts can be self-fluidized as a result of the heat produced in the particles bulk, mimicking an exothermic catalyst reaction in a chemical engineering reactor.

1. Introduction

In many industrial processes and environmental particulate flows, the assumption of isothermal flow is clearly flawed and heat exchange between the dispersed phase, i.e., the particles, and the suspending fluid might significantly alter the flow kinematics. In chemical engineering flows involving catalysts, heat is produced by the various chemical reactions taking place in the container and temperature variations of tens of kelvin are not unusual. In these cases, heat transfer dominates and controls the flow, creating natural convection currents and counter-currents, modifying locally the fluid viscosity, etc. In order to improve the various macroscopic averaged closure laws developed in the past on the base of experimental and theoretical studies, we suggest here to tackle the problem by large scale computations and direct numerical simulation (DNS). Though the introduction of heat transfer in the model is crucial to provide reliable results, only few contributions to the literature have been reported. We believe that it may be explained by the three following remarks: (i) there is still much to do to understand the physics of particulate flows in isothermal situations, (ii) the fluid/solid hydrodynamic interaction, i.e., momentum transfer, is already tough enough to model properly without adding heat transfer, (iii) this kind of computation requires a large computing power. Nevertheless, we showed (Dan & Wachs, 2010; Yu, Shao, & Wachs, 2006) that the same method employed to treat momentum transfer can easily be applied to heat transfer. In addition, remark (iii) can be overcome by the computing power offered by modern large clusters and an appropriate strategy to parallelize numerical codes, as the one we suggest in Wachs (2011).

Depending on the scale at which the flow problem is surveyed and the nature of the flow (compressible or incompressible, laminar or turbulent, etc.), different approaches are recommended. Here we investigate the heat transfer problem between the dispersed phase and the suspending fluid at the level of the particle, which implies that our method is commonly considered as a DNS one. We assume that the flow is laminar (at the level of the particle) and

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[1] Parallel Efficient LIbrary for GRains In Fluid Flow, see Wachs (2011) for details.

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incompressible. DNS methods might be classified into two families: boundary-fitted (like arbitrary Lagrangian–Eulerian (ALE) method) and non-boundary-fitted (like the Immersed Boundary (IB) method or the Distributed Lagrange Multiplier/Fictitious Domain (DLM/FD) method). We believe that the complexity of the heat transfer phenomena taking place at the fluid/solid interface coupled to the rather unpredictable motion of individual particles promotes the use of a DNS method to perform consistent numerical simulations and provide reliable results. Initially, the boundary-fitted DNS methods have been predominantly used. Gan, Chang, Feng, and Hu (2003) and Gan, Feng, and Hu (2003) simulated the sedimentation of solid particles with thermal convection using the ALE/Finite Element (FE) method. More recently, numerical simulations of particulate flows with heat transfer using a non-boundary-fitted DNS method were also reported in the literature. Kim and Choi (2004) and Pacheco, Pacheco-Vega, Rodic, and Peck (2005) developed an IB Finite Volume (FV) method for heat transfer in complex geometries without considering the motion of particles. Yu, Shao, et al. (2006) employed the DLM/FD method to solve heat transfer at the fluid/solid interface with heat conduction inside the solid bodies. Feng and Michaelides (2008, 2009a) developed an IB/FV method for heat transfer in particle laden flows under the assumption of homogeneous temperature over the particles. IB and DLM/FD methods are conceptually very similar, but the DLM/FD method has the advantage of avoiding to explicitly compute the hydrodynamic force and torque acting on particles, as well as the heat flux. In contrast, it implies to introduce two families of Lagrange multiplier (a vector-valued one for the velocity field and a scalar one for the temperature field) and to solve the resulting equations as saddle-point problems.

The DNS method advocated here to model particulate flows with heat transfer relies on a DLM/FD method, a first order operator-splitting algorithm and a FE discretization scheme. This work is an extension of the method we proposed in our previous contributions to the literature on heat transfer in particulate flows (Dan & Wachs, 2010; Yu, Shao, et al., 2006). Computations are now performed with our upgraded code, PeliGRIFF, that is able to tackle three-dimensional problems with a fair number of particles since it runs in parallel on large scale clusters. Using this new code, we investigate heat transfer situations we did not consider previously. In order to validate our solver, we compare our computed results with the data reported in various references (Feng & Michaelides, 2008, 2009; Yu, Shao, et al., 2006) on 2D problems: the settling of a single circular cylinder in a semi-infinite channel as well as an enclosure at various Grashof numbers and the rising of a single circular catalyst in an enclosure. Then, we show new results on the 3D counterpart of the 2D flow problem in an enclosure. Finally, we examine how a bed of spherical catalysts packed at the bottom of a cuboid enclosure can be self-fluidized as a result of the heat produced by an exothermic catalyst reaction on the particles, which, when transferred to the surrounding fluid, creates an upward oriented natural convection stream.

2. Simulation model

As in our previous work Yu, Shao, et al. (2006), we employ the DLM/FD method to couple the fluid and solid motion. Here we restrict heat transfer to the case of homogeneous temperature over the particle, which implies that either the solid thermal conductivity is much higher than the fluid thermal conductivity, or equivalently, that the Biot number is very small (Feng & Michaelides, 2009). This can also be seen as purely convective heat exchange between the fluid and solid phases. Finally, the fluid density varies with temperature while we assume that the fluid viscosity remains constant, the extension to temperature-dependent viscosity being straightforward. The fact that we focus here on the impact of natural convection in the fluid flow supports this approximation.

2.1. Governing equations

Let Ω be a bounded domain of $\mathbb{R}^d$, $d \in <2,3>$ and $\partial\Omega$ its boundary. Suppose that Ω is filled with N_P rigid particles $P_i(t)$, $i \in <1, N_P>$. For simplicity, we consider $N_P = 1$, the extension to the multi-body case being straightforward, and Dirichlet boundary conditions on $\partial\Omega$ for both the fluid velocity and temperature fields. Please note that we shall work with dimensionless quantities throughout the whole paper and distinguish any dimensional quantity by a "star" symbol.

Governing equations can be non-dimensionalized by introducing the following scales: L_c for length, U_c for velocity, $T_c L_c/U_c$ for time (implying that we employ a convective time scale), $\rho_f^* U_c^2$ for pressure, $\rho_f^* U_c^2/L_c$ for rigid-body motion Lagrange multiplier, $T_{s0}^* - T_{f0}^*$ for temperature and $\rho_f^* C_{pf}^* U_c (T_{s0}^* - T_{f0}^*)/L_c$ for temperature Lagrange multiplier. The variational combined conservation equations that govern both the fluid and solid motion read (Glowinski, Pan, Hesla, & Joseph, 1999; Yu, Shao, et al., 2006):

(1) Combined momentum equations

$$\int_\Omega \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)\cdot\boldsymbol{v}d\boldsymbol{x} - \int_\Omega p\nabla\cdot\boldsymbol{v}d\boldsymbol{x} + \frac{1}{\mathcal{R}e_c}\int_\Omega 2\boldsymbol{D}(\boldsymbol{u}):\boldsymbol{D}(\boldsymbol{v})d\boldsymbol{x} + \int_{P(t)} \boldsymbol{\lambda}\cdot\boldsymbol{v}d\boldsymbol{x} + \int_\Omega \frac{\mathcal{G}r}{\mathcal{R}e^2} T_f \frac{\boldsymbol{g}^*}{g^*}\cdot\boldsymbol{v}d\boldsymbol{x} = \boldsymbol{0}, \quad \forall \boldsymbol{v}\in\mathcal{V}_0(\Omega) \tag{1}$$

$$(\rho_r - 1)\left[V_P\left(\frac{d\boldsymbol{U}}{dt} - \mathcal{F}r\frac{\boldsymbol{g}^*}{g^*}\right)\cdot\boldsymbol{V} + \left(\boldsymbol{I}_P\frac{d\boldsymbol{\omega}}{dt} + \boldsymbol{\omega}\times\boldsymbol{I}_P\cdot\boldsymbol{\omega}\right)\cdot\boldsymbol{\xi}\right] - \sum_j \boldsymbol{F}_{cj}\cdot\boldsymbol{V} - \sum_j \boldsymbol{F}_{cj}\cdot\boldsymbol{\xi}\times\boldsymbol{R}_j - \int_{P(t)}\boldsymbol{\lambda}\cdot(\boldsymbol{V}+\boldsymbol{\xi}\times\boldsymbol{r})d\boldsymbol{x} + \int_{P(t)}(\rho_r\beta_r - 1)\frac{\mathcal{G}r}{\mathcal{R}e^2}T_f\frac{\boldsymbol{g}^*}{g^*}\cdot(\boldsymbol{V}+\boldsymbol{\xi}\times\boldsymbol{r})d\boldsymbol{x} = \boldsymbol{0}, \boldsymbol{V}\in\mathbb{R}^d, \boldsymbol{\xi}\in\mathbb{R}^{\tilde{d}} \tag{2}$$

$$\int_{P(t)}\boldsymbol{\alpha}\cdot(\boldsymbol{u} - (\boldsymbol{U}+\boldsymbol{\omega}\times\boldsymbol{r})d\boldsymbol{x} = 0, \quad \forall\boldsymbol{\alpha}\in\Lambda(t) \tag{3}$$

(2) Continuity equation

$$-\int_\Omega q\nabla\cdot\boldsymbol{u}d\boldsymbol{x} = 0, \quad \forall q\in\mathcal{P}_0(\Omega) \tag{4}$$

(3) Combined energy equations

$$\int_\Omega \left(\frac{T_f\partial}{\partial t} + \boldsymbol{u}\cdot\nabla T_f - Q_f\right)\cdot\Psi_f d\boldsymbol{x} + \frac{1}{\mathcal{R}e_c\mathcal{P}r}\int_\Omega \nabla T_f\cdot\nabla\Psi_f d\boldsymbol{x} + \int_{P(t)}\lambda_T\Psi_f d\boldsymbol{x} = 0, \quad \forall\Psi_f\in\mathcal{T}_0(\Omega) \tag{5}$$

$$V_P\left[(\rho_r C_{pr} - 1)\frac{dT_s}{dt} + (Q_s - Q_f)\right]\Psi_s - \int_{P(t)}\lambda_T\Psi_s d\boldsymbol{x} = 0, \quad \forall\Psi_s\in\mathbb{R} \tag{6}$$

$$\int_{P(t)}\alpha_T(T_f - T_s)d\boldsymbol{x} = 0, \quad \forall\alpha_T\in\Lambda_T(t) \tag{7}$$

where $\boldsymbol{u}\in\mathcal{V}_{\partial\Omega}(\Omega)$ denotes the fluid velocity vector, $p\in\mathcal{P}(\Omega)$ the pressure, $D = 1/2(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^t)$ the rate-of-strain tensor, $\boldsymbol{\lambda}\in\Lambda(t)$ the velocity distributed Lagrange multiplier vector, $\boldsymbol{U}\in\mathbb{R}^d$ the