International Journal of Heat and Fluid Flow 000 (2016) 1–8

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

journal homepage: www.elsevier.com/locate/ijheatfluidflow

Numerical investigation of the interaction of a finite-size particle with a tangentially moving boundary

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ARTICLE INFO

Article history:
Available online xxx

Keywords:
DG-FEM
Finite-size particle
Free-surface flow
Particle-laden flow
SPM
Wall effect

ABSTRACT

The motion of a finite-size particle in steady two-dimensional lid- and shear-driven square-cavity flows is investigated. The coupled equations are solved numerically using a discontinuous Galerkin-finite-element method (DG-FEM) combined with the so-called smoothed-profile method (SPM). The spectral convergence enables an accurate and efficient computation of particle trajectories without moving grids. Particle trajectories are obtained by solving the Navier–Stokes and Newtons's equations for the particle motion using simulations without additional model assumptions fully resolving all scales down to the flow in the lubrication gap. Particle trajectories are compared with streamlines and trajectories from one-way coupling. In the shear-driven square cavity with convex streamlines finite-size particles suffer a significant displacement effect when passing the moving boundary closely. While inertia displaces the particle towards outer streamlines, the finite-size effect alone displaces the particle towards inner streamlines. For weakly inertial particles the latter displacement effect is shown to be qualitatively similar to the displacement modelled by inelastic collision in a one-way-coupling approach.

1. Introduction

Two-phase flows arise in many natural phenomena and are of great interest for industrial processes (Crowe et al., 2011). Therefore, it is of crucial importance to understand the basic mechanisms involved in such flows in order to predict and control their behaviour.

Among multiphase flows, particle-laden flows are made of a connected fluid phase and an immiscible dispersed phase consisting of particles. Typically, the particles are very small compared to the reference length of the fluid domain in which they are immersed. If, in addition, liquid volume displaced by the particulate phase is small, i.e. the particle volume fraction is $\phi < 0.001$, the particles can be considered point particles (Crowe et al., 2011). In addition, some models also neglect the feedback of the (point) particles on the fluid flow which significantly simplifies the numerical treatment. The assumption of point particles which do not affect the fluid motion leads to a one-way coupling between the fluid and the particle phase. However, the one-way-coupling approximation must necessarily break down if a particle moves close to a boundary of the domain (a wall or a free-surface) within a distance of the order of the particle size. Thus, near the boundaries the finite particle size can play an important role in the evolution of the particulate phase.

An example in which the motion near a free surface plays a crucial role is the rapid clustering of particles into so-called particle accumulation structures (PAS) (Schwabe et al., 1996; 2007). Since the particle accumulation also takes place in very dilute suspensions (Tanaka et al., 2006), the numerical modeling to date was based on the hypothesis that the particle accumulation is a single-particle phenomenon such that particle–particle interactions have been neglected. However, as demonstrated by Hofmann and Kuhlmann (2011) and Mukin and Kuhlmann (2013), particle–boundary interactions cannot be neglected. In fact, the particle–boundary interaction was shown to be of crucial importance for PAS. To model this interaction (Hofmann and Kuhlmann, 2011) have suggested an inelastic collision model, also called particle–free-surface interaction (PSI) model (Mukin and Kuhlmann, 2013), which is based on a single interaction-length parameter. Even though the PSI model can semi-quantitatively predict the shape of PAS in its final time-asymptotic state, the model cannot correctly describe the temporal evolution of the accumulation process. Obviously, this deficit is due to the discontinuous ad-hoc assumptions entering the PSI model. Moreover, employing the PSI model along with an inappropriate interaction-length parameter may fake a particle-accumulation which does not physically exist in corresponding experiments.

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http://dx.doi.org/10.1016/j.ijheatfluidflow.2016.07.011
0142-727X/© 2016 Published by Elsevier Inc.

While the PSI model is computationally very efficient, it is not based on first principles and it is lacking in several respects. On the other hand, a fully-resolved approach without any further modeling is feasible for a single particle phenomenon. The fully-resolved simulation would enable (a) a prediction of the dynamical evolution of the attraction of a single particle to a limit cycle (PAS), (b) a numerical proof or disproof of the existence of PAS for specific flow conditions, and (c) it would yield the correct interaction-length parameter to be used in the computationally more economic one-way coupling approach.

The aim of the present investigation, therefore, is to remedy the inconsistency of the one-way-coupling approach in combination with the PSI model by accurately investigating the effect of tangentially moving walls and free-surfaces on the trajectories of finite-size particles immersed in an incompressible fluid flow. The flow systems targeted are relevant for PAS, because the streamline crowding near the moving boundaries significantly enhances the probability and thus the importance of particle–boundary interactions.

Several two- and four-way coupled simulations have been carried out employing rebound schemes to deal with particle–boundary and particle–particle interactions (see e.g., Ardekani and Rangel (2008)). Here, we go a step further and directly simulate the particle–boundary interaction, based only on the Navier–Stokes equations and Newton's law without any further modeling. To that end the flow will be fully resolved on all relevant scales, including the lubrication flow in the thin gap between the particle and the boundary. This direct approach makes rebound models dispensable.

The problem is mathematically formulated in Section 2. Section 3 describes the discretization method using DG-FEM and SPM, including some benchmarks to verify the correct implementation of the numerical solver. Section 4 gathers the results of a parametric investigation. The effect of inertia and of an initial velocity-mismatch on the particle–wall and particle–free-surface interactions are presented. The results are then compared with those of the discontinuous PSI model (Hofmann and Kuhlmann, 2011; Kuhlmann and Hofmann, 2011). Finally, in Section 5, conclusions will be drawn and perspectives for future investigations are outlined.

2. Formulation of the problem

We consider the transport of solid particles in an incompressible Newtonian fluid. For simplicity we neglect buoyancy forces. The governing equations are the Navier–Stokes equations valid in the fluid phase

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1a}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \boldsymbol{u}, \tag{1b}$$

$$\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T = \kappa \nabla^2 T, \tag{1c}$$

and Newton's equations of motion for the ith particle moving in the fluid

$$\boldsymbol{F}_i = M_i \dot{\boldsymbol{V}}_i, \tag{2a}$$

$$\boldsymbol{R}_i = \mathsf{I}_i \cdot \dot{\boldsymbol{\Omega}}_i, \tag{2b}$$

where ρ_f is the fluid density, $\boldsymbol{u}$, p and T are the flow velocity, pressure and temperature field, respectively, ν is the kinematic viscosity, κ the thermal diffusivity, and $\boldsymbol{F}$, $\boldsymbol{R}$, $\boldsymbol{V}$, $\boldsymbol{\Omega}$, M and I are the particles forces, torques, translational and rotational velocities, mass and inertia tensor, respectively. The coupling between the two phases results from the no-slip condition on the particle surfaces.

While the equations of motion have been presented in a dimensional form, the flow simulation employs a non-dimensionalization. Since we shall consider the pure mechanical lid-driven cavity and also a thermocapillary-driven cavity we apply different scalings depending on the particular case. For the lid-driven cavity we use the convective scaling

$$\boldsymbol{u} = \hat{\boldsymbol{u}} U, \quad \boldsymbol{x} = \hat{\boldsymbol{x}} L, \quad t = \hat{t} \frac{L}{U} \quad , \quad p = \hat{p} \rho_f U^2, \tag{3}$$

where U is the velocity of the lid, L a characteristic length, and the superscript $\hat{}$ indicates non-dimensional quantities. For the thermocapillary-driven cavity we use the viscous scaling

$$\boldsymbol{u} = \hat{\boldsymbol{u}} \frac{\nu}{L}, \ \boldsymbol{x} = \hat{\boldsymbol{x}} L, \ t = \hat{t} \frac{L^2}{\nu}, \ p = \hat{p} \frac{\rho_f \nu^2}{L^2}, \ T = \hat{T} \Delta T, \tag{4}$$

where ΔT is a characteristic temperature difference.

3. Numerical methods and code validation

The numerical treatment of two-phase problems can be roughly classified into two main categories. In the Lagrangian description of the particle motion a computational mesh is co-moving with the particle (e.g. the arbitrary Lagrangian-Eulerian (ALE) method (Duarte et al., 2004)). In the Eulerian representation of the particle motion all governing equations are solved on a stationary grid (distributed Lagrange multiplier, DLM, force coupling method, FCM, immersed boundary method, IMB and immersed interface method, IIM, see e.g. Lomholt and Maxey (2003) and Peskin (2002)).

In the present investigation, an Eulerian approach is adopted implementing a *smoothed-profile method* (SPM). It includes the effect of the particles on the flow in a smooth body-force fashion instead of explicitly enforcing the no-slip boundary condition on the particles' surfaces. The computational grid for the flow simulation covers both phases. In order to include the influence of the particulate-phase on the flow field a smooth body force is added to the momentum Eq. (1)b. Such a body-force is defined via a thin interface layer across each particle surface which is used to smoothly pass from fluid-dynamics to rigid-body equations of motion.

To calculate the velocities of the particles we use the penalty-body-force approach as discussed in Luo et al. (2009) and Nakayama and Yamamoto (2005). This method guarantees the rigidity of the particle and implicitly applies the no-slip boundary condition responsible for coupling the two-phases. To distinguish between the solid domain of particle i and the surrounding fluid domain we use the concentration function

$$\phi_i(\boldsymbol{x}, t) = \frac{1}{2}\left[\tanh\left(\frac{a_i - |\boldsymbol{x} - \boldsymbol{P}_i|}{\xi_i}\right) + 1\right], \tag{5}$$

where $\boldsymbol{P}_i$ and ξ_i are, respectively, the centroid position and the interface thickness of the ith particle and a_i is the radius of the particle assumed to be circular (in 2D) or spherical (in 3D). The function ϕ is called the *smoothed profile* and equals to one inside the particles, whereas it is zero in the fluid phase. For temporal discretization the second-order stiffly-stable splitting scheme of Karniadakis et al. (1991) is employed, including a semi-implicit treatment of the particle-phase. For the spatial discretization we use a discrete-Galerkin finite-element method (DG–FEM). Within this approach the algorithm used for simulating the particle-laden flow (1) and (2) reads (see Luo et al., 2009 for details)

$$\boldsymbol{P}_i^{n+1} = \boldsymbol{P}_i^n + \Delta t \sum_{k=0}^{K} a_k \boldsymbol{V}_i^{n-k}, \tag{6a}$$

$$\frac{\delta_0 \tilde{\boldsymbol{u}} - \alpha_0 \boldsymbol{u}^n - \alpha_1 \boldsymbol{u}^{n-1}}{\Delta t} = -\beta_0 \boldsymbol{N}(\boldsymbol{u}^n, \boldsymbol{u}^n) - \beta_1 \boldsymbol{N}(\boldsymbol{u}^{n-1}, \boldsymbol{u}^{n-1}), \tag{6b}$$

Please cite this article as: F. Romanò, H.C. Kuhlmann, Numerical investigation of the interaction of a finite-size particle with a tangentially moving boundary, International Journal of Heat and Fluid Flow (2016), http://dx.doi.org/10.1016/j.ijheatfluidflow.2016.07.011