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Analysis of unsteady Lagrangian and Eulerian characteristics of a liquid fluidized bed by Direct Numerical Simulation.

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Abstract

The characterization of fluidized beds is still a challenging task for macroscopic modeling issues and industrial applications. The macroscopic models require to be fed with parameters or laws that are not well understood or even impossible to estimate as soon as the solid fraction is larger than 0.1. The aim of the present work is to investigate Direct Numerical Simulation [1] of unsteady particle flows in order to solve all the time and space scale of the flow and the particle and to allow for the estimate of unknown macroscopic or stochastic characteristics of the flow. In the DNS, the particles are fully resolved, i.e. the particle diameter is larger than the grid size and to the smallest hydrodynamic scale. A benchmark experimental fluidized bed [2] is simulated and analyzed in terms of macroscopic and Lagrangian characteristics. Comparisons of numerical solutions to measurements are achieved with success.

keywords: DNS of fluidized bed, resolved scale particles, viscous penalty method

1 Introduction

The characterization of dense liquid-solid flows and in particular fluidized beds is still a challenging task for macroscopic modeling issues and industrial applications as the granular dynamics based models or scale separation Eulerian-Eulerian or Eulerian-Lagrangian approaches. These macroscopic models require to be fed with parameters or laws that are not well understood or even impossible to estimate as soon as the solid fraction is larger than 0.1. The aim of the present work is to investigate Direct Numerical Simulation [1] of unsteady particle flows in order to solve all the time and space scale of the flow and the particle and to allow for the estimate of unknown macroscopic or stochastic characteristics of the flow. In the DNS, the particles are fully resolved, i.e. the particle diameter is larger than the grid size and to the smallest hydrodynamic scale.

Simulating a fluidized bed where particle and fluid have the same characteristic scales, *i.e.* resolved scale particle flows, is the scope of the present work. The Direct Point Simulation (DPS) approaches based on a Lagrangian modeling of the particles does not remain valid for that purpose [3] [4] [5]. The field of numerical methods devoted to the simulation of particulate flows involving finite size particles was widely developed the last 20 years concerning the study of the flow over a small number of fixed or moving particle [6] [7] [8] [9] [10] [11] or a fixed arrangement of spheres [12]. All the previously mentioned works were developed on fixed grids. The unstructured Arbitrary Eulerian-Lagrangian (ALE) grid simulations were developed for particle flows in the 90's by Hu *et al.* [6] concerning two-dimensional flows involving two particles. The works of Maury [13] with the ALE method are also to be noticed concerning the flow of 1000 non spherical particles in a two-dimensional biperiodic domain. A majority of the particulate flow simulations were carried out on structured grids to avoid the complexity of managing an evolving adapted mesh. Among them, the most relevant existing works concern the distributed Lagrangian multiplier (DLM) method of Glowinski and co-workers [14], the Physalis CFD code of Zhang and Prosperetti [15], the Immersed Boundary (IB) with direct forcing approach proposed by Uhlmann [16] [17], the lattice Boltzmann scheme [18, 19], the modified version of Uhlmann IB method published by Lucci *et al.* [20] [21] and the viscous penalty techniques of Ritz and Caltagirone [22] and Ranzani *et al.* [23] [24] [1]. The present work uses the second order in space penalty method for the DNS of particulate flows based on the Implicit Tensorial Penalty Method [1].

2 Simulation of real fluidized bed

2.1 Presentation of the fluidized bed

The fluidized bed chosen for the simulations is taken from the experiments of Aguilar Corona [2]. In a cylinder of $0.64m$ height and $0.08m$ diameter, 2133 pyrex particles are fluidized by the circulation of potassium thiocyanate KSCN at various fluidization velocities. The diameter of the particles is $0.006m$ and the simulated fluidization velocity is $0.12m.s^{-1}$. The density of the pyrex is $\rho_s = 2230 kg.m^{-3}$ whereas the density ρ_l and the dynamic viscosity μ_l of the KSCN are $1400 kg.m^{-3}$ and $3.8 \cdot 10^{-3} Pa.s$. For the chosen particles in KSCN, the terminal settling velocity is equal to $0.226 m.s^{-1}$, the particle Reynolds number based on this velocity is equal to 530 and the Stokes number is 0.8. Concerning the DNS of particles, a parallelepiped box of dimensions $8 cm \times 8 cm \times 64 cm$ is used with a grid mesh containing $160 \times 160 \times 1280$ cells. With such a grid resolution, nearly 12 cell length Δx per particle diameter is achieved. The cylinder is penalized by a Darcy technique [25].

2.2 Macroscopic results

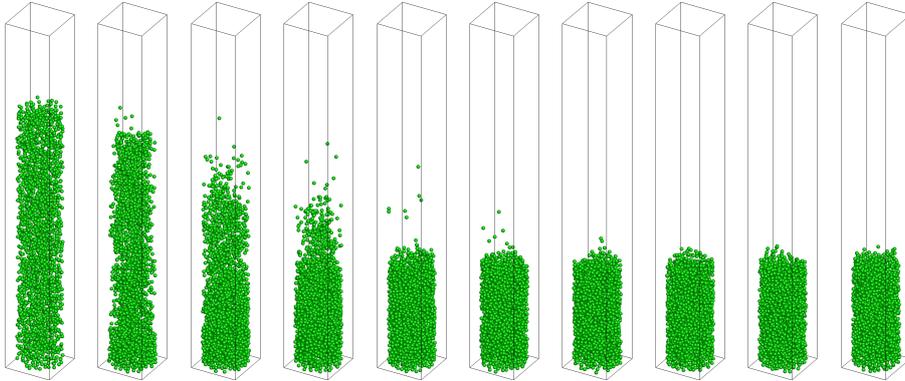


Figure 1: Three-dimensional view of the particles inside the fluidized bed - from left to right, $t = 1, 2, 3, 4, 5, 6, 7, 8, 9$ and $10s$.

The macroscopic characteristics of the fluidized bed are first presented in order to validate the global interaction between the 2133 particles and the carrier fluid. The typical particle structures are illustrated in figure 1 over time. It is observed that from $t = 0s$ to $6s$, a packing occurs as the initial particle concentration α , *i. e.* $\alpha = 0.1$, is small compared to the fluidization velocity of $0.12m.s^{-1}$. After $6s$, the fluidization regime is reached and the average bed height and resulting solid concentration in the vertical cylinder remain almost constant over time. The average numerical solid

concentration α_n so obtained is 0.24. For the chosen operating conditions, this value of α_n can be compared to the reference experimental correlation of Richardson and Zaki [26] which reads

$$\alpha_{RZ} = 1 - \left(\frac{U_0}{U_t} \right)^{1/2.41} \quad (1)$$

where the parameter 2.41 is correct for Reynolds numbers Re_t based on the settling particle velocity larger than 500. In our configuration, $Re_t = 530$. Concerning the fluidization velocity U_0 and the settling particle velocity U_t , the values of $0.12m.s^{-1}$ and $0.226m.s^{-1}$ are measured in the experiments of [2]. Finally, it is found that $\alpha_{RZ} = 0.231$. A very good agreement is found between experiments and numerical solutions. This comparison validates the use of two numerical radii for the particles, one for the definition of the density and the treatment of the collisions and the other for the penalty viscosity. A correct global equilibrium between the gravity and drag forces is so obtained.

2.3 Lagrangian characteristics

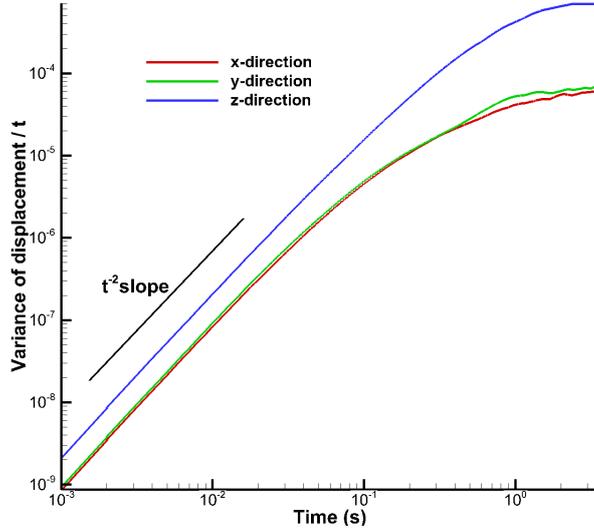


Figure 2: Variance of the displacement of the particles $\frac{M_{\alpha\alpha}}{t}$ according to time.

The first Lagrangian characteristics that can be studied are the particle velocity fluctuations over time in the fluidization regime, for $t > 6s$. In this particular flow conditions, the mean particle positions are null as the height of the bed height is constant over time. The numerically measured time averaged particle velocities are $\bar{U}_x = 7.2150 \cdot 10^{-5}m.s^{-1}$, $\bar{U}_y = 7.7822 \cdot 10^{-5}m.s^{-1}$

and $\bar{U}_z = 1.4128 \cdot 10^{-5} m.s^{-1}$ respectively in the x , y and z directions. These values are four orders of magnitude smaller than the fluidization velocity and can be considered as zero.

| | x-direction | y-direction | z-direction |
|-------------------------------------|-----------------------|----------------------|----------------------|
| experiments of [2] ($m^2.s^{-1}$) | 5.4×10^{-5} | 5.1×10^{-5} | 6.8×10^{-4} |
| simulations ($m^2.s^{-1}$) | 4.55×10^{-5} | 5.5×10^{-5} | 7.5×10^{-4} |

Table 1: Asymptotic values of $\frac{M_{\alpha\alpha}(t)}{t}$ for each Cartesian direction.

A last parameter of interest to feed the macroscopic Eulerian-Eulerian models devoted to fluidized beds is the autodiffusion coefficient $D_{\alpha\alpha}$. It is defined [2] according to the variance of the particle displacement $M_{\alpha\alpha} = \langle \mathbf{X}_i - \mathbf{X}_{i,0} \rangle$ as

$$D_{\alpha\alpha} = \lim_{t-t_0 \rightarrow +\infty} \frac{M_{\alpha\alpha}(t)}{t} \quad (2)$$

where \mathbf{X}_i is the coordinate vector of one particle at a given time step and $\mathbf{X}_{i,0}$ is the coordinate vector of the same particle at an initial time t_0 . The notation $\langle \cdot \rangle$ stands for the average over all the particles $i, i = 1..2133$. In the experiments [2], it has been demonstrated that for small time steps, a t^{-2} slope was observed for $D_{\alpha\alpha}$ whereas an asymptotic value was reached for larger times. This asymptotic value is the autodiffusion coefficient in a given direction. The curve of $\frac{M_{\alpha\alpha}(t)}{t}$ is presented in figure 2. The same slope as in the experiments is found numerically for small time steps. The asymptotic values obtained numerically and in the experiments for $D_{\alpha\alpha}$ are proposed in table 1. A good agreement is found between experiments and numerical solutions, the vertical component being one order of magnitude larger than in the horizontal directions. A 16% gap is observed between both approaches.

3 Conclusion and perspectives

A fictitious domain approach based on augmented Lagrangian techniques and penalty methods has been used for handling particulate flows of resolved scale particle. The work has been concentrated on the simulation of a real fluidized bed, in order to illustrate the ability of the ITPM to deal with dense particulate flows. The simulations have been favorably compared to reference experiments or theoretical results of the literature such as the fluidization velocity, variance of particle position or auto-diffusion coefficient. These simulations are a first step for managing numerical experiments with

the DNS of particle flows. This is now possible on massively parallel computers, as 512 processors were used in the proposed simulations of fluidized beds.

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