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3D numerical simulation of a lab-scale pressurized dense fluidized bed focussing on the effect of the particle-particle restitution coefficient and particle–wall boundary conditions

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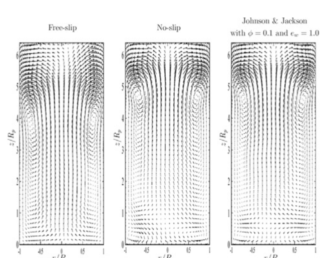
HIGHLIGHTS

- Comparison between time-averaged Euler particle velocity profiles and PEPT results.
- Prediction of double toroidal recirculation loops for large solid wall shear stress.
- Testing of No-slip wall boundary condition for Euler particle velocity.

GRAPHICAL ABSTRACT



Effect of wall boundary condition for solid phase on the time-averaged solid velocity field

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ABSTRACT

3D numerical simulations of dense pressurized fluidized bed are presented. The numerical prediction of the mean vertical solid velocity are compared with experimental data obtained from Positron Emission Particle Tracking. The results show that in the core of the reactor the numerical simulations are in accordance with the experimental data. The time-averaged particle velocity field exhibits a large-scale toroidal (donut shape) circulation loop. Two families of boundary conditions for the solid phase are used: rough wall boundary conditions (Johnson and Jackson, 1987 and No-slip) and smooth wall boundary conditions (Sakiz and Simonin, 1999 and Free-slip). Rough wall boundary conditions may lead to larger values of bed height with flat smooth wall boundary conditions and are in better agreement with the experimental data in the near-wall region. No-slip or Johnson and Jackson's wall boundary conditions, with sufficiently large value of the specularity coefficient ($\phi \geq 0.1$), lead to two counter rotating macroscopic toroidal loops whereas with smooth wall boundary conditions only one large macroscopic loop is observed. The effect of the particle-particle restitution coefficient on the dynamic behaviour of fluidized bed is analysed. Decreasing the restitution coefficient tends to increase the formation of bubbles and, consequently, to reduce the bed expansion.

1. Introduction

Pressurized gas–solid fluidized beds are used in a wide range of industrial applications such as coal combustion, catalytic polymerization, uranium fluoration and biomass pyrolysis. The mathematical modelling and numerical simulation of such industrial fluidized beds are challenging because many complex phenomena

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are in competition (particle–turbulence interaction, particle–particle and particle–wall collisions, heat and mass transfers) and because of the large-scale geometry of the industrial facilities compared to the characteristic length scales of the fluid and particles.

The development of numerical modelling of dense fluidized bed hydrodynamics started about three decades ago (Gidaspow, 1994). Basically two approaches can be used for the numerical prediction of dense fluidized bed hydrodynamic: the Euler-Lagrange approach, where filtered Navier–Stokes equations are solved for the gas and Discrete Element Method (DEM) for the particles (Kaneko et al., 1999; Deen et al., 2007; DiRenzo and Di Maio, 2007; Olaofe et al., 2014), or the multi–fluid approach where all phases are treated as continuum media. In the DEM approach, the Lagrangian trajectories of each particle are computed and the inter–particle collisions are treated in a deterministic manner. Even if DEM can be used up to a few millions of particles (Capecelatro and Desjardins, 2013) it cannot yet be used for most of industrial full-scale simulations. Typically, to simulate the lab-scale fluidized bed studied in the present paper, the whole number of particles to be accounted for in the frame of the DEM approach is about 10 millions while for an industrial pressurized gas-phase olefin polymerization reactor (Neau et al., 2013) the corresponding number of particles should be larger than 40 billions. In contrast, nowadays it is possible to perform realistic 3D simulations of industrial configurations by using an unsteady Eulerian reactive multi-fluid approach. Numerical simulations of industrial-, pilot- and lab-scale pressurized reactors were carried out with such an approach showing a good agreement with the qualitative knowledge of the process but detailed experimental validations were missing (Gobin et al., 2003; Fede et al., 2010; Rokkam et al., 2010; Fede et al., 2011a, 2011b; Rokkam et al., 2013). Indeed, the Euler–Euler approach is extensively used for circulating or dense gas-solid fluidized bed predictions but the model assessment is commonly restricted to a comparison between the predicted and the experimentally measured pressure drop, or local mass flux. Obviously such restrictions come from the complexity of doing measurements inside a dense particulate phase. Recently, an original experimental technique, called Positron Emission Particle Tracking (PEPT), has emerged allowing to measure the trajectory of an individual particle moving in dense particulate flows. From the trajectory it is possible to compute the particle dispersion properties and then to perform fruitful comparison between experiments and numerical prediction (Link et al., 2008; Fede et al., 2009).

The present paper shows numerical results from Euler–Euler simulations carried out with the mathematical model proposed by Balzer et al. (1995) (see Appendix A). Such a modelling approach involves several assumptions however there is no empirical constant in the model. In fact the model, like all Lagrangian or Eulerian ones, requires the value of the normal restitution coefficient for particle-particle collision. Precisely speaking, the normal restitution coefficient is not an adjustable parameter because it represents the physical loss of kinetic energy during a collision. However, as this parameter is very difficult to measure for a practical powder (Foerster et al., 1994; Sommerfeld and Huber, 1999), it can be seen as a parameter of the modelling approach (Goldschmidt et al., 2001). In the present paper a comprehensive analysis is made for showing how the normal restitution coefficient may modify the macroscopic properties of a dense fluidized bed.

In the framework of the kinetic theory of dry granular flows, several wall boundary conditions for the solid phase have been derived for rough or flat walls, with or without frictional effect (Hui et al., 1984; Johnson and Jackson, 1987; Jenkins and Richman, 1986; Jenkins, 1992; Jenkins and Louge, 1997; Sakiz and Simonin, 1999; Konan et al., 2006b; Schneiderbauer et al., 2012; Soleimani et al., 2015). For the numerical simulation of a circulating or dense fluidized bed the most popular wall boundary conditions are the ones derived by Johnson and Jackson (1987) which introduced a specularity coefficient that is an ad-hoc parameter depending on the large-scale roughness of the walls but which cannot be measured directly from experiment, in contrast to the normal restitution coefficient (Sommerfeld and Huber, 1999). In the case of dilute gas-solid flow in a pipe, Benyahia et al. (2005) showed that the specularity coefficient must be very small for correct agreement with experimental data. Li et al. (2010) analysed the effect of the specularity coefficient on the predicted 2D and 3D hydrodynamic of dense bubbling fluidized beds. Unfortunately, the 3D study considered only small values of the specularity coefficient ranging from 0.0 to 0.05. In parallel, wall boundary conditions have been derived for flat frictional walls (Jenkins and Richman, 1986; Jenkins, 1992; Louge, 1994; Jenkins and Louge, 1997; Sakiz and Simonin, 1999; Schneiderbauer et al., 2012). The development and validation of such boundary conditions were mainly performed by comparison with predictions from the Discrete Element Method (DEM).

It is important to note that the original Johnson and Jackson boundary conditions do not account for particle/wall frictional effects. In contrast, the more recent boundary conditions of Konan et al. (2006a, 2006b) and Soleimani et al. (2015) extend different approaches, originally developed for smooth walls, by using the idea of virtual wall angle of Sommerfeld and Huber (1999).

The paper is organized as follows. The second section gives an overview of the experiment where the PEPT technique was used for obtaining local statistics of the solid inside the fluidized bed. The boundary conditions for the solid phase employed in the present study are described in the third section. The description of the numerical simulation, in terms of equations, mesh, material properties and statistics are given in the fourth section. The results are presented in section five and, finally, an analysis is carried out in section six on the specific dependence of the simulation results on the particle-particle collision restitution coefficient and on the solid wall boundary conditions. Conclusions and prospects are given in the last section.

2. Experimental overview

This study concerns the hydrodynamics of an isothermal gas-solid dense fluidized bed in a low-scale pressurized axisymmetric reactor with a cylindrical column of internal radius $R = 77$ mm and height 1 074 mm (see Fig. 1). The vertical distance between the horizontal gas fluidization distributor plate and the widening (with an enlargement half-angle of 10°) is 924 mm. Nitrogen enters at the distribution plate with a fluidization velocity $V_f = 0.32$ m/s and the pressure in the fluidized bed is 12 bar. The gas and solid material properties are given in Table 1. The particle phase is almost monodisperse with a median diameter of 875 µm and a material density of 740 kg/m^3.

Positron Emission Particle Tracking (PEPT) is an experimental technique developed at the University of Birmingham derived from the medical imaging method Positron Emission Tomography (PET) (Stellema et al., 1998). PEPT enables the tracking of a single particle in an opaque or otherwise impenetrable system such as dense fluidized beds. PEPT tracers are labelled with a specific class of radioisotope which decays through the emission of a positron (β^+ decay). The emitted positron collides with a local electron, annihilates and produces a pair of back-to-back gamma photons. The usual isotope is Fluorine-18; this has excellent characteristics of decaying solely through β^+, is easily manufactured by Helium-3 ion irradiation of oxygen-containing materials such as water or