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EFFECT OF WALL BOUNDARY CONDITIONS AND MESH REFINEMENT ON NUMERICAL SIMULATION OF PRESSURIZED DENSE FLUIDIZED BED FOR POLYMERIZATION REACTOR

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ABSTRACT
The effect of the mesh refinement and the solid phase boundary condition are investigated for numerical simulation of dense pressurized fluidized bed. Two fluidized beds have been considered: a laboratory-scale device and a pilot-scale facility. A relation is proposed to scale-up the numerical simulation and preserving the spatial resolution accuracy. As expected the boundary condition of the solid phase modifies the behaviour of the fluidized bed. Compared to free-slip wall boundary condition, a no-slip condition improves the numerical predictions with respect to available experimental data.

INTRODUCTION
Pressurized gas-solid fluidized beds are used in a wide range of industrial applications such as coal combustion, catalytic polymerization, uranium fluoration or biomass pyrolysis. The numerical modelling of such industrial fluidized beds is challenging because many complex phenomena take place (particle-turbulence interaction, particle-particle and particle-wall collision, heat and mass transfers) and the large-scale geometry of the industrial facilities. The development of numerical modelling of fluidized bed hydrodynamic started about two decades ago. Nowadays it is possible to perform 3D realistic simulations of industrial configurations by using unsteady Eulerian reactive multi-fluid approach. Numerical simulations of industrial and pilot-reactor were carried out with such an approach showing a good agreement with the qualitative knowledge of the process (bed height, pressure drop, local mass flux). However the size of industrial reactor and the computer resources imposed too coarse meshes. Recent studies have emphasized the role of the spatial resolution on the prediction of the fluidized bed behaviour (Agrawal et al (1); Igci et al (2); Parmentier et al (3-4)). Also it has been shown that for dilute (Benyahia et al (5)) and dense (Fede et al (6)) gas-solid flow the boundary condition of the solid phase may modify the structure of the flow. According to Fede et al (6), in dense fluidized bed, the no-slip wall boundary improves the prediction of the radial profile of mean vertical particle velocity compared to the results predicted by using a free-slip wall boundary condition.

In the present study, 3D numerical simulations of dense pressurized fluidized beds have been carried out using an Eulerian n-fluid modelling approach for fluid-particle turbulent polydispersed flows developed and implemented by IMFT (Institut de Mécanique des Fluides de Toulouse) in the NEPTUNE CFD V1.07@Tlse version.

Table. 1. Mesh characteristics for laboratory- and pilot-scale reactors.

			Laboratory-scale		Pilot-scale	
Diameter	D_r	(m)	0.077		0.74	
Height	H_r	(m)	1.7		9.1	
Cell number			80 245	384 156	217 668	1 636 032
	dx/D_r	(-)	0.037	0.016	0.018	0.009
	dz/D_r	(-)	0.068	0.068	0.054	0.027

NEPTUNE CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA (Commissariat à l'Energie Atomique), EDF (Electricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA-NP.

The multiphase Eulerian approach is derived from a joint fluid-particle PDF equation allowing to derive the transport equations for the particle velocity's moment (Simonin (7)). In the proposed modelling approach, separate mean transport equations (mass, momentum, and fluctuating kinetic energy) are solved for each phase and coupled through inter-phase transfer terms. The drag law is modified according to Gobin et al (8). The collisional particle stress tensor is derived in the frame of the kinetic theory of granular media (Boëlle et al (9)). The turbulence modelling is achieved by the standard $k-\varepsilon$ model extended to the multiphase flows (i.e. accounting for additional source terms due to the inter-phase interactions). For the dispersed phase, a coupled transport equation system is solved on particle fluctuating kinetic energy and fluid-particle fluctuating velocity covariance (Simonin (7)).

In the present paper, we analyze the effect of the solid wall boundary conditions and mesh size for several fluidized bed systems: first a laboratory-scale bed (0.9m of height) and a pilot-scale bed (9m of height). The numerical simulation of an industrial-scale bed (34m of height) is discussed and the results will be shown at the conference.

GEOMETRY, MESH AND SCALING

The numerical simulations were carried out for several isothermal reactors: first a laboratory-scale reactor with a diameter of 0.077m and an height of 1.7m, second a pilot-scale device with a diameter of 0.74m and a height about 9 meters. For the comparison, simulations were carried out for an industrial-scale polymer reactor has a diameter of 5m and a height of 34m.

In the last few years, the sensitivity of the numerical simulation with respect to the mesh has been investigated. Agrawal et al (1) showed that a very fine mesh (typically with a cell size of the order of a few particle diameters) permits to capture some meso-scale structures. These structures have a strong influence on the hydrodynamic of the fluidized bed especially on the bed height, on the vertical solid mass flux and the mixing process. Recent studies (Heynderickx et al (10); Igci et al (2)) pointed out the role of the drag force in the formation of the meso-scales. These studies were made by a priori analysis of mesh-independent numerical simulation.

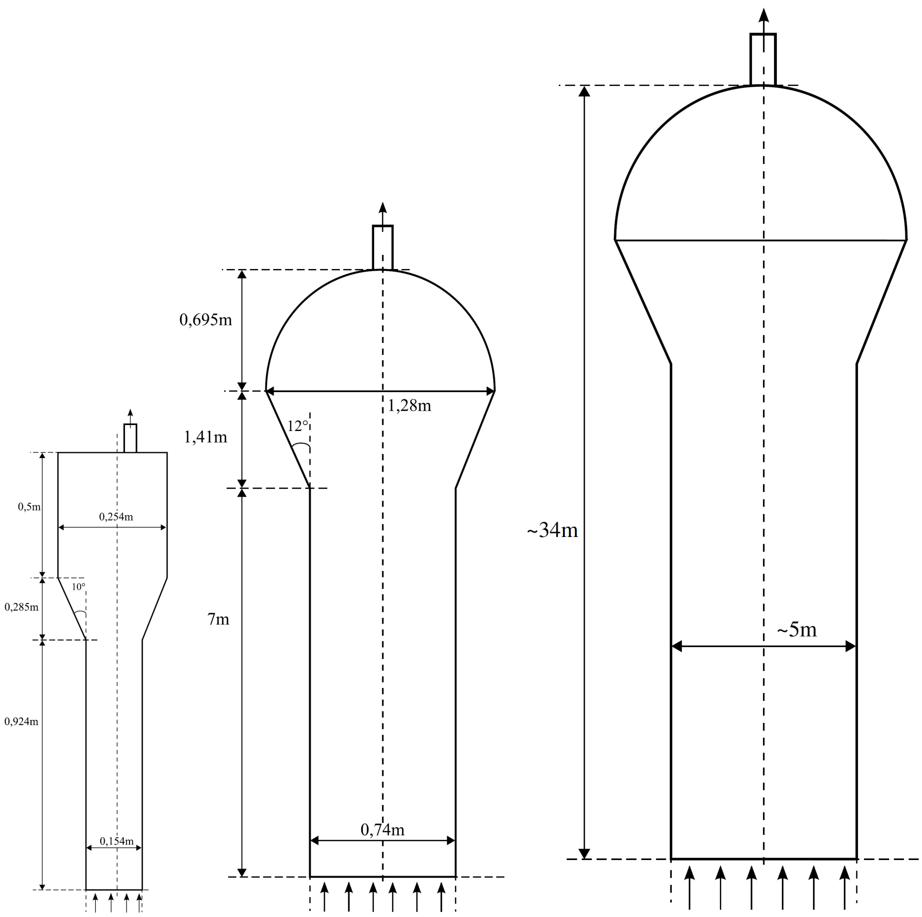

Fig. 1. Sketches of the reactor. From the left to the right: the laboratory-scale reactor, the pilot-scale reactor and the large industrial facilities.

Parmentier et al (3) have shown that the error related to the mesh can be scaled. Indeed, for similar operating conditions and particle properties, considering a numerical simulation of a dense fluidized bed of diameter D_r with a cell size of Δ, the required mesh for a larger reactor of diameter $\tilde{D}_r$ and conserving the error due to the mesh is given by:

$$\tilde{\Delta} = \Delta \sqrt{\tilde{D}_r / D_r} \qquad (1)$$

The meshes have been constructed using O-grid technique in order to have nearly uniform cells in a horizontal section ($dx \approx dy$). The Table 1, giving the main characteristics of the meshes for the laboratory- and pilot-scale reactors, shows that the cell size dx is nearly in accordance with Equation (1) when passing from the laboratory-scale to the pilot-scale reactors.

The numerical simulations are performed in two steps. First the column of the fluidized bed is filled of solid. The solid volume fraction is uniformly distributed and determined in order to fit the solid mass of the experiment. Then a transitory phase, corresponding to the destabilization of the bed, is computed during 20 seconds (the

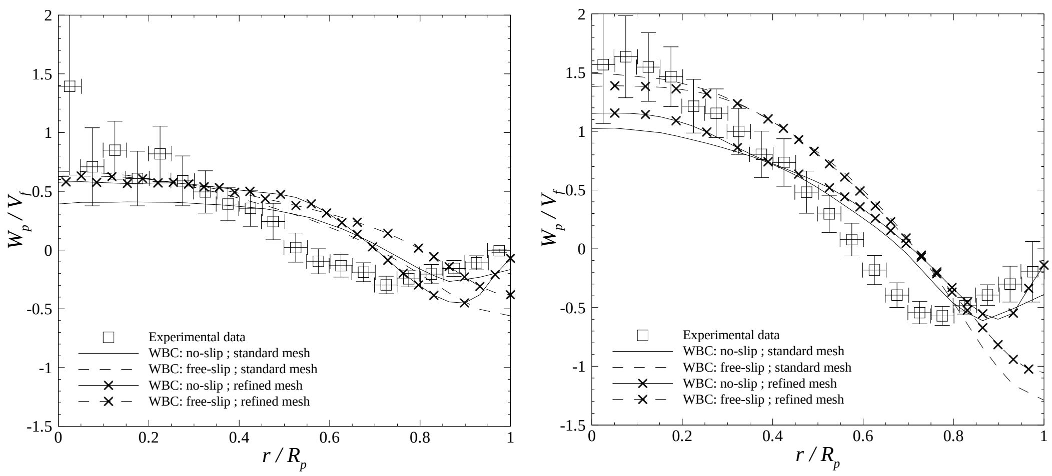

Fig. 2. Laboratory-scale: radial profile of the mean vertical particle velocity normalized by the fluidization velocity (V_f). The operating pressure is P=12bar and the fluidization velocity V_f=0.32m/s. On the left-panel the data has been extracted at $z=0.75\times D_r$ and the right panel $z=1.7\times D_r$.

time step is approximately 10^{-3}s). In a second step, the time-averaged statistics are computed during 80s in order to obtain converged statistics.

LABORATORY-SCALE DEVICE

The experimental investigation of dense fluidized bed is a trickiest challenge. Because of the medium opacity, the experimental data are commonly reduced to pressure drop at the wall or local solid mass flux. However, recently a novel technique has been developed called Positron Emission Particle Tracking allowing to access to the local properties of the solid flow. This non-invasive technique consists of tracking a single particle (up to now it is possible to have multiple particle tracking) and using specific algorithm to reconstruct the Lagrangian trajectory of the particle inside the fluidized bed. This technique has been successfully employed to investigate the hydrodynamic of dense fluidized bed (Link et al (11); Fede et al (6)). The drawback of the PEPT method is that the entire reactor has to be equipped of sensor. Then, the using of PEPT to investigate an industrial reactor is still quite complicated. However the PEPT can be used on a laboratory-scale fluidized bed. Such experimental works are crucial to improve the knowledge on the local mechanisms taking place in a fluidized bed. This is also relevant to assess a modelling approach and closure laws used in Euler-Euler models.

Fede et al (6) made an analysis of experimental data obtained by PEPT. On the radial profiles of the time-averaged mean vertical particle velocity they observed that in the near-wall region the solid velocity is nearly equal to zero. It suggests that a no-slip wall boundary condition for the solid phase is more suitable than a free-slip condition. However, a no-slip boundary condition for the mean particle velocity and zero flux for the particle fluctuating kinetic energy are very questionable but could represent elastic bouncing on the wall with an isotropic angle distribution. Such a situation could correspond to spherical particles bouncing on very rough wall or to

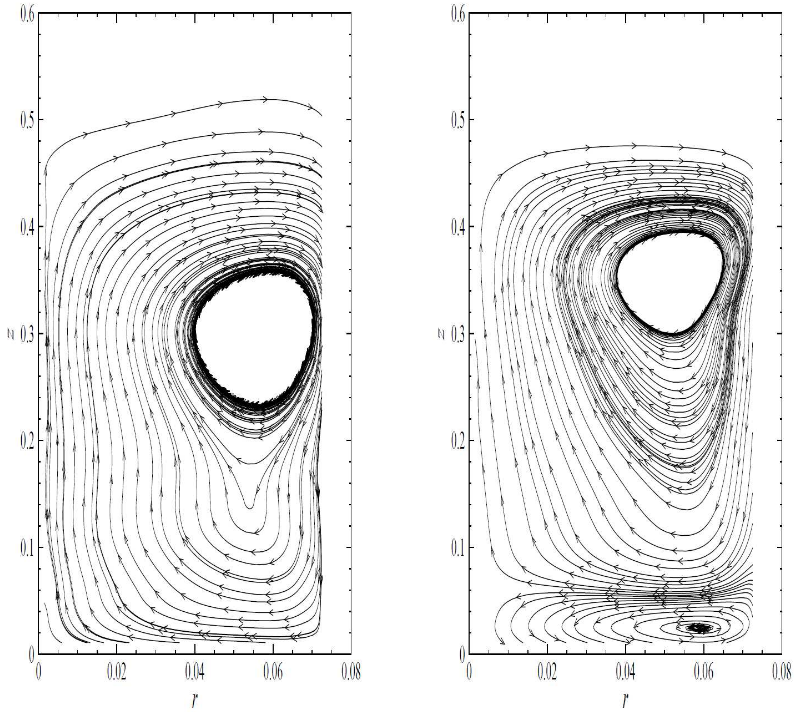

Fig. 3. Pilot-scale: streamtraces of the time-averaged simulated particle velocity. Left panel: free-slip wall boundary condition for solid phase, right-panel: no-slip boundary condition. The operating pressure is P=12 *bar* and the fluidization velocity V_f=0.32m/s.

very irregular particles bouncing on a smooth wall (Konan et al (12)). However the experimental observations have shown a downward solid flux at the wall. Then one may emphasize that wall boundary condition for the mean solid velocity is between the free-slip and the no-slip condition.

The Figure 2 shows the radial profile of the time-averaged mean vertical particle velocity using the two meshes and both boundary condition. The operating pressure is 12bar and the fluidization velocity 32cm/s and the particles are Geldart's B type. As shown by Figure 3 such a dense pressurized fluidized bed exhibits a peculiar hydrodynamic with a 3-dimensional recirculating loop. The figure shows that the modification of the wall boundary condition for the mean particle velocity changes the topology of the flow. The free-slip condition leads to a one-loop system whereas a no-slip boundary condition to a two counter-rotating recirculating loop. The recirculating loop is clearly shown by the radial profiles in Figure 2. Indeed, we observe an upward mean vertical particle velocity at the bed centre (r = 0) and in the near-wall region a downward particle velocity. We observe that the mesh refinement does not have a significant effect on the time-averaged mean particle vertical velocity. In contrast, the Figure 3 shows that the no-slip wall boundary condition gives the same trend than the experimental data. In particular, the slope break appearing close to wall is well predicted even if the position of the slope break is not correct. Similar trends have been observed with the same particles but differing in terms of fluidization velocity and operating gas density.

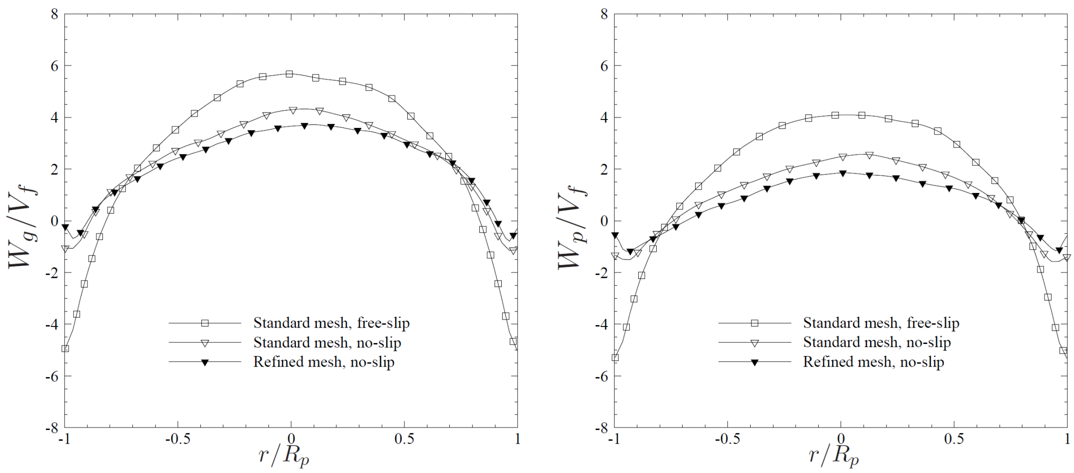

Fig. 4. Pilot-scale: radial profile of the time-averaged mean vertical gas (left) and solid (right) velocity normalized by the fluidization velocity. The radial profile is extracted at $z=3.2\times D_r$.

PILOT-SCALE FACILITY

The pilot-scale reactor investigation is particularly important because the operating conditions are very close to the ones in industrial process. In addition, the flow simulation conditions of such a device are well controlled (in terms of temperature, velocity of fluidisation, particle properties) and experimental data are available (pressure drops, temperature, gas composition).

Fede et al (13) performed numerical simulations of such a polymerization pilot reactor located at INEOS Lavéra (France). As for the laboratory-scale they found a large recirculating loop. The Figure 4 shows the radial profile of the time-averaged mean vertical gas and solid velocity in the pilot-scale fluidized bed. We observe that the structure of the flow is similar to the one observed in the laboratory-scale reactor. Namely, we notice a large upward particle velocity at the reactor centre (up to 4 times the fluidisation velocity) and a downward particle velocity near the wall. This typical profile indicates the presence of the recirculating loop. The figure 4 shows that the profile of the gas velocity profile has the same shape than the profile of the particle velocity. In such a fluidized bed, the near-wall region is characterized by large downward solid mass flux. Then, the particles drag the gas in their motion leading to negative vertical gas velocity. The modification of the wall-boundary condition for the solid phase clearly modifies this effect. Indeed, Figure 4 exhibits a strong reduction of the downward particle velocity at the wall and consequently a reduction of the downward gas velocity. The mass conservation leads to decrease the particle velocity at the reactor centre.

The vertical mean pressure distribution is shown by Figure 5. The pressure distribution exhibits a slope break corresponding to the top of the fluidized bed. With the free-slip wall boundary condition the pressure distribution inside the fluidized bed is found slightly bended whereas a no-slip condition gives linear profiles. This effect may be explained by the recirculating loop identified in such a fluidized bed. Indeed, the free-slip boundary condition should lead to a too large rotating motion of the

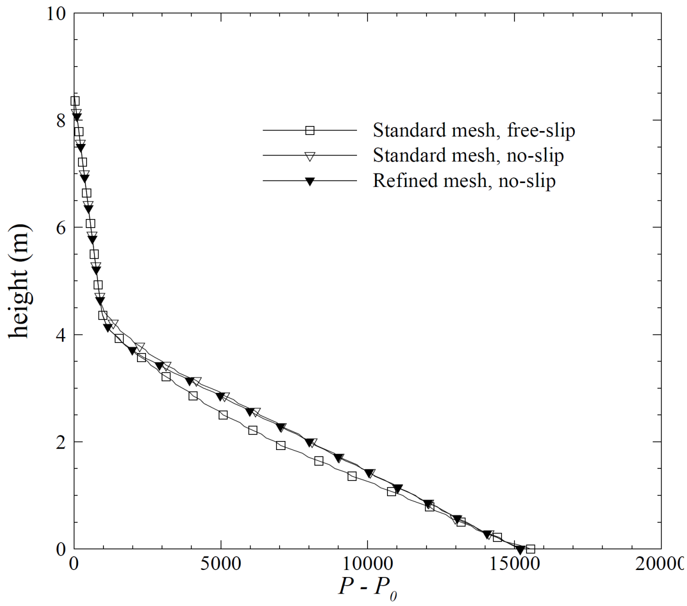

Fig. 5. Vertical mean gas pressure distribution measured at the wall in pilot-scale reactor.

recirculating loop. Then, the gas and the particles are accelerated at the centre of the bed modifying the pressure distribution. The mesh refinement does not significantly modify the pressure distribution even if the top of the fluidized bed is slightly decreased with the mesh refinement. It was expected because the particles correspond to Geldart's B particle type. For such kind of particles the sensitivity of the numerical solution with the mesh is less important than for Geldart's A particles.

INDUSTRIAL-SCALE FACILITY

In the two previous sections, we have briefly described the hydrodynamic of isothermal laboratory-scale and pilot-scale device. For the considered operating points and powder properties, Equation (1) gives the required mesh size to ensure a good spatial resolution. If we apply such a scaling-rule, the mesh for the industrial-scale configuration requires about 4,000,000 cells. Nowadays such a numerical simulation is realizable using High Parallel Computing. In particular the parallel efficiency of NEPTUNE CFD has been demonstrated up to 1,024 CPU (Neau et al (14)). Such an industrial-scale numerical simulation is currently running and the results will be presented.

CONCLUSION

Numerical simulations of pressurized dense fluidized bed for polymerization have been carried out and compared with experimental data for laboratory-scale and pilot scale. The effect of boundary conditions on the solid phase has been investigated and the results show that the prediction of the gas pressure vertical distribution is improved with a no-slip boundary condition for the mean solid velocity.

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NOTATION

D_r	diameter of the reactor	W_g	mean vertical gas velocity
H_r	height of the reactor	W_p	mean vertical solid velocity
V_f	operating fluidization velocity	P	gas pressure

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