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Acceleration of inertial particles in wall bounded flows: DNS and LES with stochastic modelling of the subgrid acceleration

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Abstract. Inertial particle acceleration statistics are analyzed using DNS for turbulent channel flow. Along with effects recognized in homogeneous isotropic turbulence, an additional effect is observed due to high and low speed vortical structures aligned with the channel wall. In response to those structures, particles with moderate inertia experience strong longitudinal acceleration variations. DNS is also used in order to assess LES-SSAM (Subgrid Stochastic Acceleration Model), in which an approximation to the instantaneous non-filtered velocity field is given by simulation of both, filtered and residual, accelerations. This approach allow to have access to the intermittency of the flow at subgrid scale. Advantages of LES-SSAM in predicting particle dynamics in the channel flow at a high Reynolds number are shown.

1. Introduction

Understanding the Lagrangian behaviour of inertial particles in turbulent channel flows has important implications for many environmental systems, from sediment transport to atmospheric dispersion of pollutants or solid deposition in marine flows. Previous experimental (Kaftori *et al.*, 1995) and numerical (Marchioli & Soldati, 2002) studies on particle-laden channel flows have examined particle deposition, trapping, segregation or the modification of particle velocity statistics due to the presence of coherent structures. It is recognized that inertial effects cause particle segregation and clustering (Kiger & Pan, 2002). As shown by Bec *et al.* (2006) or Ayyalasomayajula *et al.* (2008) for a high Reynolds number “free” turbulence, these phenomena are connected with particle acceleration statistics. In our paper, such statistics are of interest in the case of a high Reynolds number channel flow. This may help in understanding and modelling complex interactions between particle dynamics and wall flow structures.

Lagrangian measurements of Ayyalasomayajula *et al.* (2008) Qureshi *et al.* (2008) and Gerashchenko *et al.* (2008) or computations of Marchioli & Soldati (2002) and Lavezzo *et al.* (2010) provided insight into inertial particle accelerations and their statistics, including the acceleration probability density functions (PDF), in both homogeneous and inhomogeneous flows. These studies showed that, in the case of homogeneous isotropic turbulence, solid particles with low inertia exhibit highly non-Gaussian acceleration PDF with a high probability of intense acceleration events. These acceleration PDF tend to narrow and to gaussianize as particles inertia increases as shown by Bec *et al.* (2006). These authors suggested that the trend

of acceleration PDF to gaussianity, as well as a monotonic decrease of acceleration variance, are both a consequence of preferential concentration (dominant at small Stokes numbers) and filtering (for particles with larger Stokes numbers).

One could expect the same tendencies in the presence of the wall: preferential concentration and filtering may decrease the variance of particle acceleration. However, close to the wall, the flow is very different from homogeneous isotropic turbulence. There are typical streaks, aligned with the wall, characterized by alternating high and low longitudinal speed regions. Low inertia particles do not see this alternation of regions; once such particles get trapped in the structure, they travel with it. Highly inertial particles do not respond to this intermittency neither, due to the filtering effect. Only particles with intermediate inertia may respond to the spanwise alternation of high and low speed regions; this may cause an additional agitation of those particles. In this paper, particle acceleration statistics in the channel flow are explored, in comparison with the effects described by Bec *et al.* (2006) for the case of homogeneous isotropic turbulence.

For single phase flows, large-eddy simulation (LES) has become a suitable tool that produces acceptable results at much lower computational costs than direct numerical simulation (DNS). However, application of LES in turbulent channel flow becomes too expensive when the Reynolds number is high and the resolution of strong subgrid gradients is needed. An alternative to standard LES, referred to as LES-SSAM approach was proposed by Sabel'nikov *et al.* (2007, 2011). In this approach, the exact Navier-Stokes equation is replaced by a model equation in which the instantaneous total acceleration is viewed as a sum of two model accelerations. One represents the filtered acceleration closed by eddy viscosity model, the other one emulates the residual (subgrid) acceleration. The later is done by two independent stochastic processes, for the norm of this acceleration and for its orientation. For the turbulent channel flow a new stochastic model for the subgrid acceleration was proposed by Zamansky *et al.* (2010), and was assessed in the case of turbulent channel flow in the framework of LES-SSAM approach.

Such a development of LES-SSAM approach (Zamansky *et al.*, 2010) is further applied to particle-laden channel flows in this paper. The advantages of the method will be tested in regard of particle velocity and acceleration statistics. Results will be compared with DNS and classical LES. The tests will be run for different types of particles given by Stokes numbers from 1 to 125.

The article is organized as follows. In the next section, the numerical method is briefly described. Then, we present some results obtained by DNS concerning particle acceleration as well as fluid acceleration as seen by particle. In the last section, the LES-SSAM approach is compared to DNS and classical LES. Finally, conclusions are stated.

2. Numerical method

2.1. Flow

The flow considered is an incompressible turbulent channel flow. Periodic boundary conditions are imposed on the fluid velocity field in x (streamwise) and z (transverse) directions and no-slip boundary conditions are imposed at the walls.

Three different sets of numerical simulations for the fluid are treated here: direct numerical simulation of channel flow (DNS), standard large-eddy simulation (LES) and large-eddy simulation coupled with stochastic forcing of subgrid acceleration (LES-SSAM). For the cases of LES and LES-SSAM the classical Smagorinsky model is used (Sagaut, 2002).

Details on the simulation characteristics are summarized in Table 1. In the following the superscript “+” denotes quantities expressed in wall units. For the three simulations, the Reynolds number based on the u_τ , the channel half height h and ν , is set to $Re_\tau = 587$.

Table 1. Simulation parameters. N_i , L_i and Δ_i are the number of grid points, the domain length and the grid spacing in direction i , respectively.

| Type | Re_τ | Re | $N_x \times N_y \times N_z$ | $L_x \times L_y \times L_z$ | $\Delta x^+ \times \Delta y^+ \times \Delta z^+$ |
|----------|-----------|-------|-----------------------------|--------------------------------------|--|
| DNS | 587 | 12490 | $384 \times 257 \times 384$ | $3/2\pi h \times 2h \times 3/4\pi h$ | $7.2 \times (0.04 \sim 7.2) \times 3.6$ |
| LES | 587 | 14160 | $64 \times 65 \times 64$ | $3\pi h \times 2h \times \pi h$ | $87 \times (0.71 \sim 29) \times 29$ |
| LES-SSAM | 587 | 12760 | $64 \times 65 \times 64$ | $3\pi h \times 2h \times \pi h$ | $87 \times (0.71 \sim 29) \times 29$ |

The incompressible Navier-Stokes equations in a turbulent channel flow are solved using a Galerkin spectral approximation (Fourier Chebyshev) and a variational projection method on a divergence free space Buffat *et al.* (2011). Steady state fluid statistics have been compared with other DNS in Zamansky *et al.* (2010).

2.2. Particles

Particle-particle interactions are neglected as well as gravity or the influence of particles on the carrier fluid. Mirror conditions are applied for particle-wall bouncing. Furthermore, particles are considered to be point-wise, spherical, rigid and to obey the following Lagrangian dimensionless equation of motion :

$$\begin{aligned} \frac{d\vec{v}_p}{dt} &= \frac{1}{St} (\vec{u} - \vec{v}_p) f(Re_p) \\ \frac{d\vec{x}_p}{dt} &= \vec{v}_p. \end{aligned} \quad (1)$$

Here, \vec{v}_p and \vec{x}_p are the dimensionless particle velocity and position. The solid particle - fluid interaction is modelled by a drag force with the correction term $f(Re_p) = 1 + 0.15Re_p^{0.687}$ suggested by Clift *et al.* (1978). Re_p is the local and instantaneous particle Reynolds number based on the local relative velocity, the particle diameter d_p and the fluid viscosity. St is the Stokes number given by :

$$St = \frac{\tau_p}{\tau_f}, \quad (2)$$

with $\tau_p = \frac{\rho_p d_p^2}{18\rho\nu}$ and $\tau_f = \frac{\nu}{u_\tau^2}$, ρ_p and ρ being respectively the particle and fluid density. Five sets of particles are considered with $St = 1$, $St = 5$, $St = 15$, $St = 25$ and $St = 125$. For each set we used $\rho_p/\rho = 770$

A high order three dimensional Hermite interpolation is used for computing the fluid velocity $\vec{u}(\vec{x}_p, t)$ at the particle position. The time-integration of the particle motion (equation 1) is performed using a second-order Adams-Bashforth method with the same time step as the DNS. Once the particles released, the simulations are run over several particle timescales τ_p . Particle statistics are sampled starting from $t^+ \sim 1000$, counted from particle release. It has been checked that for all simulations, velocity statistics for the solid phase are at stationary state.

In this study, the acceleration is evaluated using the velocity time derivative along particle trajectories. Even though we use a three dimensional Hermite interpolation for computing the fluid velocity at particle position, as suggested by Choi *et al.* (2004) numerical errors are generated when a particle crosses a grid point. Therefore, as Mordant *et al.* (2004), the acceleration is estimated by a convolution of the Lagrangian velocity with the derivative of a

Gaussian kernel. This ensures both time derivation and filtering. The filter width, of the order of Kolmogorov time scale at the wall, is such that there is agreement between fluid Lagrangian and Eulerian acceleration 1-point statistics.

In the case of DNS, Vinkovic *et al.* (2011) have compared particle velocity statistics with the benchmark Marchioli *et al.* (2008) for a lower Reynolds number, and with experiments of Lelouvetel *et al.* (2009) for higher Reynolds numbers.

3. DNS acceleration statistics

In this section we present some results obtained by DNS.

3.1. Acceleration variance

Figure 1 shows the longitudinal acceleration variance of solid particles as a function of $y^+ = yu_\tau/\nu$. Far from the wall (say $y^+ > 50$) it is seen that as particle inertia increases the acceleration variance departs from the fluid and decrease monotonically. This is in accordance with previous studies in homogeneous isotropic flows (Bec *et al.*, 2006; Ayyalasomayajula *et al.*, 2008; Calzavarini *et al.*, 2009) and results from the simultaneous effect of preferential concentration and filtering. However in the near wall region ($y^+ < 50$) the evolution of the variance is no more monotone. For $St = 5$, the longitudinal acceleration variance presents the highest peak close to the wall. This peak is even higher than the fluid longitudinal acceleration variance. This is a clear departure that observation made for homogeneous isotropic turbulence. To gain insight on this behaviour, we analyze the acceleration statistics of the fluid seen by the solid particles.

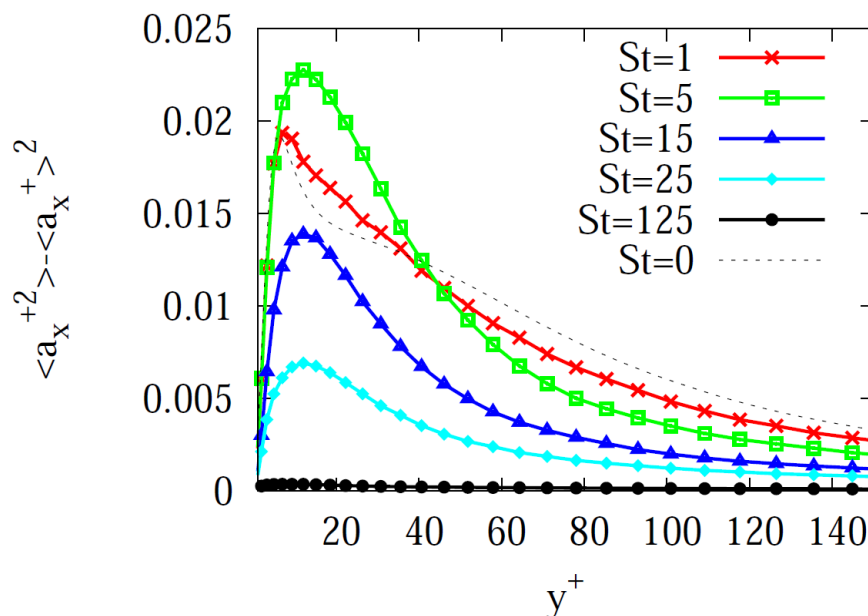


Figure 1. Longitudinal acceleration variance profile for solid particles with different Stokes numbers and for the fluid ($St = 0$).

Figure 2 illustrates the profile of longitudinal acceleration variance of the fluid conditioned at the solid particles position. The variance for the fluid seen by the solid particles is higher than the variance of the non-conditioned fluid. This is especially the case close to the wall, at

the position of the peak of longitudinal acceleration variance. The peak of fluid longitudinal acceleration at the solid particle position increases as the Stokes number increases. Whereas, as seen in figure 1, the peak of solid particle acceleration first increases from $St = 1$ to $St = 5$ and then decreases as the Stokes number further increases.

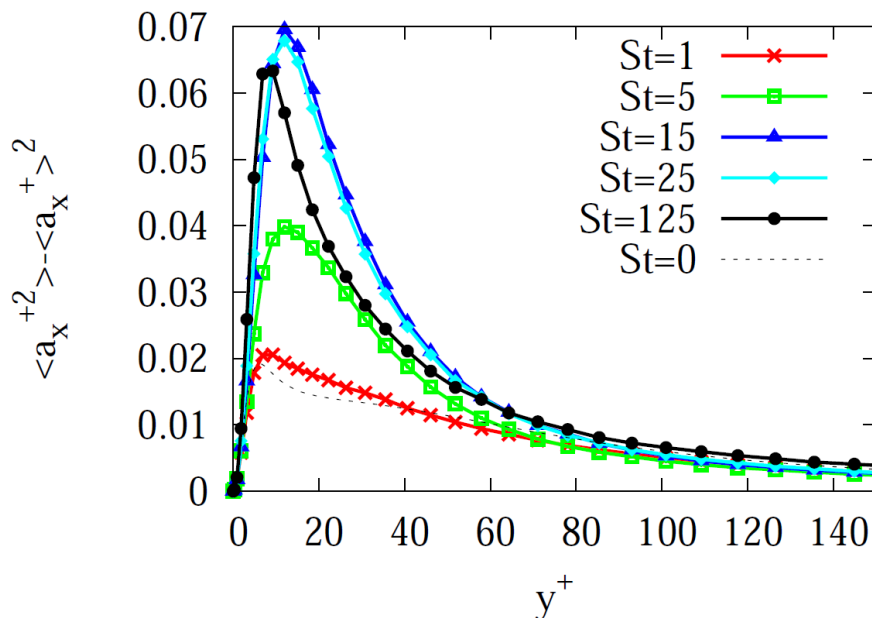


Figure 2. Longitudinal acceleration variance profile for the fluid seen by the solid particles with different Stokes numbers and for the fluid ($St = 0$).

These observations suggest that in the case of wall bounded flow, solid particles are entrained preferentially by regions with relatively high longitudinal acceleration variance. The contrary is observed in homogeneous isotropic turbulence (Bec *et al.*, 2006; Ayyalasomayajula *et al.*, 2008; Calzavarini *et al.*, 2009), where previous studies found that inertial particles tend to cluster in regions of the fluid experiencing relatively low fluid accelerations. This effect is assumed to be due to the random alternation of high and low speed streaks. Wall bounded flows present spatial alternation of high and low speed vortical structures aligned with the channel wall. As in homogeneous isotropic turbulence, inertial particles are ejected from high vorticity regions toward high strain (high dissipation rate) regions. Inertial particles are swept by these regions and due to the random alternation of high and low speed streaks, inertial particles see fluid with high longitudinal acceleration variance. Slightly inertial particles (with a response time τ_p similar to the characteristic fluid time scale) may well respond to the fluid solicitations and therefore experience an increase of their longitudinal acceleration variance. Whereas, due to the filtering effect of inertia, very inertial particles ignore the wall turbulent structures and therefore present a more homogeneous concentration and a lower acceleration variance.

3.2. Acceleration PDF

In Figure 3 we compare the normalized PDFs of longitudinal and vertical acceleration, respectively, at $y^+ \sim 100$ for different Stokes numbers with the normalized PDFs obtained by using the fluid acceleration on the particle position. For reference, the normalized PDF for the non-conditional fluid acceleration is plotted as well. As expected, when the Stokes number increases, the tails of the normalized solid particle PDFs become narrower. For all Stokes

numbers, the normalized PDFs of the fluid seen by the solid particles overlap almost perfectly with the normalized PDFs of the non-conditional fluid. The same conclusions can be drawn for other distances to the wall and for the transverse component of the acceleration. For sake of brevity, these plots are not shown here. The overlap suggests similarity of structure in terms of statistical distribution of fluid acceleration seen by the solid particles. The scaling factor is given by the acceleration RMS, which is different for each Stokes number.

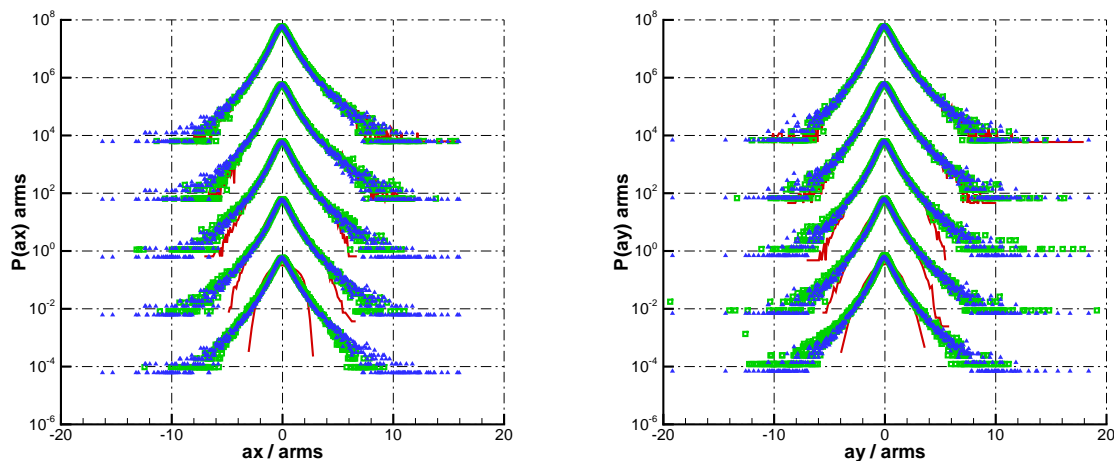


Figure 3. Longitudinal(a) and vertical (b) acceleration PDF at $y^+ = 100$, for (from top to bottom) $St = 1, 5, 15, 25, 125$. Solid particles (line), fluid particles (triangle), fluid seen by solid particles (square).

These results emphasize the significance of fluid acceleration statistics on particle dynamic. In the frame of LES, because structures are under-resolved, there is no access to small scale fluid acceleration. In the next section, LES is coupled with a stochastic model for subgrid acceleration in order to reproduce the flow intermittency at subgrid scales.

4. LES-SSAM applied to particles

Here we briefly describe the stochastic subgrid model for the acceleration used in the LES-SSAM approach. The LES-SSAM is then compared to classical LES and DNS in the case of particle laden turbulent channel flows.

4.1. LES-SSAM approach

In order to take into account the non-resolved acceleration in standard LES, the approach proposed in Sabel'nikov *et al.* (2007, 2011) is used here. In this approach, the total instantaneous acceleration is given by two contributions : $a_i = \bar{a}_i + a'_i$. The first component is the filtered total acceleration where the overbar denotes the filtering operation. The second component represents the total acceleration in the residual field. When both parts are modelled, their sum gives an approximation to the instantaneous non-filtered velocity field.

In the case of the channel flow, a model for the subgrid acceleration was proposed in Zamansky *et al.* (2010). In this model, the norm of the subgrid acceleration is simulated stochastically, using statistical universalities in fragmentation under scaling symmetry (Gorokhovski & Saveliev, 2008) in order to represent the long range interaction across the channel. The acceleration

orientation is also simulated stochastically as a random walk on a unit sphere. Starting from an orientation parallel to the wall, at the wall, this model provide relaxation toward isotropy with increasing the distance to the wall. Both stochastic models are considered as independent processes.

In comparison with standard LES, it was showed that the LES-SSAM approach gives better prediction of velocity statistics (mean and RMS profiles as well as spectra), turbulent and viscous stresses and is able to reproduce the stretched tails of fluid acceleration PDFs.

In the following section, we apply this model to the case a of particle laden channel flow.

4.2. Results and comparisons

Figure 4 show the solid particle mean and RMS velocity profiles obtained from the LES-SSAM model and compared to the DNS and LES results. The LES-SSAM model gives a better estimation of the mean solid particle velocity than classical LES (Figure 4a). In addition to this, there is also an improvement of the prediction of the vertical velocity RMS profile (Figure 4b).

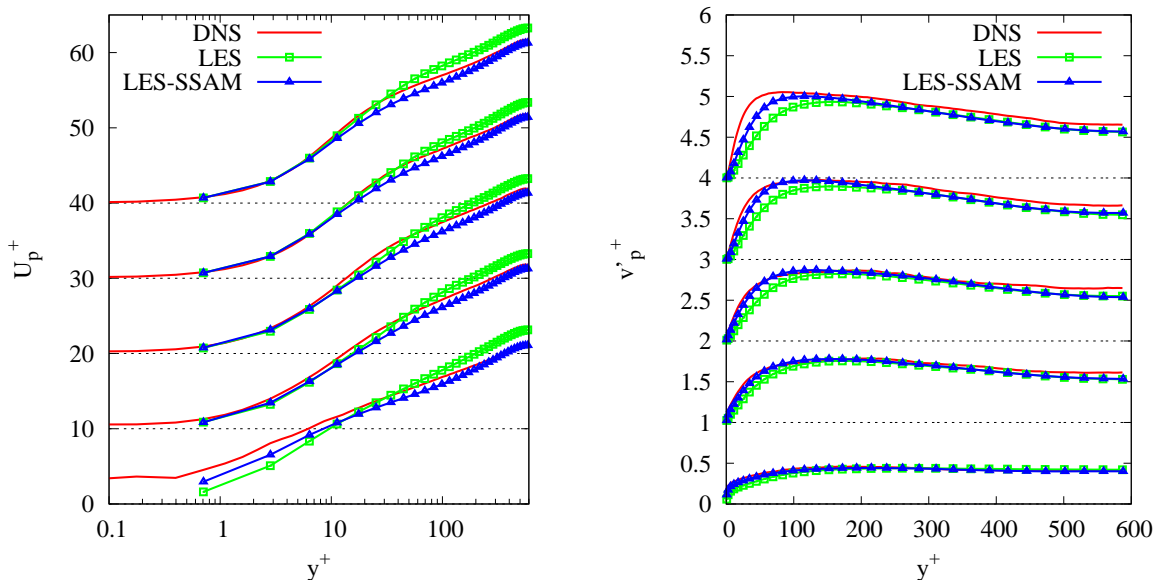


Figure 4. Mean longitudinal velocity profile (a) and vertical velocity RMS profile (b) of solid particles for (from top to bottom) $St = 1, 5, 15, 25, 125$. DNS (line), LES (squares), LES-SSAM (triangles).

Figures 5 illustrate the RMS for the transverse component of the solid particle acceleration. The evolution with St and y^+ is well reproduced by LES-SSAM, while standard LES predicts much lower values of the acceleration RMS. For other components of the acceleration we observe either the same improvement either no difference with classical LES. These results point out the importance of predicting subgrid scale acceleration for estimating solid particle velocity and acceleration statistics.

5. Conclusion

In this study, numerical simulations of particle laden turbulent channel flow are performed for five different Stokes numbers and a moderate Reynolds number. Acceleration statistics obtained

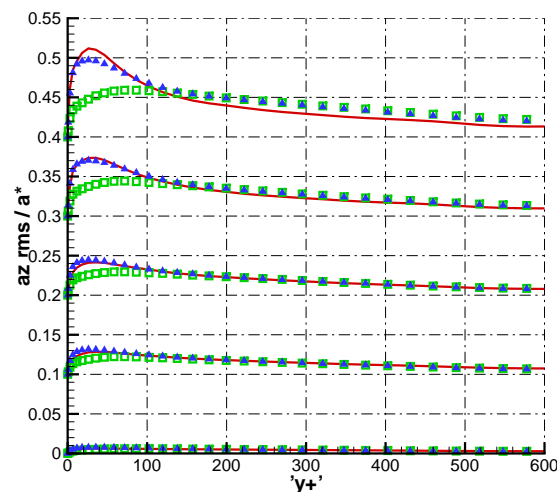


Figure 5. Transverse acceleration RMS profile of solid particles for (from top to bottom) $St = 1, 5, 15, 25, 125$. DNS (line), LES (squares), LES-SSAM (triangles).

by DNS show that in wall bounded flows, effects predicted in homogeneous isotropic turbulence by Bec *et al.* (2006) are completed by a new aspect which is additional agitation of particles by random alternation of high and low speed streaks. Depending on their inertia particles may well respond to those fluid solicitations (experiencing an increase of the longitudinal acceleration variance) or ignore the wall turbulent structures (presenting in that case a more homogeneous concentration).

In order to introduce the intermittency of structure at subgrid scale a model for the subgrid acceleration in turbulent channel flow have been introduced by Zamansky *et al.* (2010) in the framework of LES-SSAM (Sabel'nikov *et al.*, 2007, 2011). The capability of LES-SSAM for particle-laden turbulent channel flow is assessed by comparing the results with DNS and classical LES. The LES-SSAM model gives a better estimation of the solid particle velocity and acceleration statistics. This demonstrate the relevance of the LES-SSAM approach for simulations of multiphase flow at a high Reynolds number when significant physics taking place on subgrid scales. In future studies, the LES-SSAM approach will be applied to the simulation of vaporization, and cavitation in two-phase flows.

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