LARGE EDDY SIMULATION OF THE DISPERSION OF SOLID PARTICLES IN A TURBULENT BOUNDARY LAYER

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ABSTRACT

A large eddy simulation (LES) with the dynamic Smagorinsky-Germano subgrid-scale (SGS) model is used to study the dispersion of solid particles in a turbulent boundary layer. Solid particles are tracked in a Lagrangian way. The resolution of the Lagrangian equation of the solid particle motion requires the knowledge of the instantaneous velocity of the surrounding fluid. This velocity is considered to have a large-scale part (directly computed by the LES) and a small-scale part. The subgrid-scale velocity of the surrounding fluid is given by a three-dimensional Langevin model. The stochastic model is written in terms of SGS statistics at a mesh level. In addition to this, an appropriate Lagrangian correlation timescale is considered in order to include the influences of gravity and inertia of the solid particle. The results of the LES are compared with the wind-tunnel experiments of Nalpanis et al. (1993 *J. Fluid Mech.* **251** 661-685) and of Taniere et al. (1997 *Exp. in Fluids* **23** 463-471) on sand particles in saltation and in modified saltation, respectively, over a flat bed. Our simulations predict the quantitative features of both experiments.

INTRODUCTION

The entrainment, transport and deposition of dust-sized sediment can have a severe impact on the natural environment and human activity. For a sufficiently strong wind, dust particles can be entrained by aerodynamic forces of by the impact forces of saltating grains which return to the soil and interact energetically. This last phenomenon is considered as the main source of dust particle entrainment and erosion (Shao et al. 1993).

Owing to an increasing interest in environmental problems, considerable attention has been focused on the prediction of sand particle motion in atmospheric turbulent boundary layers. Since the pioneering work of Deardorff (1970), LES has become a well established tool for the study of turbulent flows (Meneveau and Katz, 2000) as well as the transport of solid particles in a variety of conditions (Wang and Squires, 1996; Shao and Li, 1999). However, since only the motion of the large scales is computed, the effect of the small scales on particle dispersion, motion or deposition must be either modeled separately or neglected. In this study, a modified Lagrangian stochastic model is coupled with a LES with the dynamic Smagorinsky-Germano SGS model (Germano et al., 1991), in order to take into account the SGS motion of particles.

The subgrid-scale velocity of solid particles is given by a modified three-dimensional Langevin model, which is written in terms of the local SGS characteristics. This way, the Lagrangian stochastic model is entirely given by the quantities directly computed by the LES with the dynamic Smagorinsky-Germano SGS model, Germano et al. (1991). A modified Lagrangian correlation timescale is considered in order to include the influences of gravity and inertia of the solid particle. In addition to this, inter-particle collisions and two-way coupling are introduced.

The results of the computations are compared with the wind-tunnel experiments of Nalpanis et al. (1993) and of Taniere et al. (1997) on sand particles in saltation and modified saltation, respectively, over a flat bed.

LARGE-EDDY SIMULATION

A turbulent boundary layer flow is computed using the LES code ARPS 4.5.2. Details of the resolved equations and subgrid closure are given in Aguirre et al. (2005). The continuity and momentum equations obtained by grid filtering the Navier-Stokes equations are:

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0 \ ,$$
$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \tau^r_{ij}\right) + \tilde{B}_i \ , \quad (1)$$

where u_i is the fluid velocity, p is the total pressure, ν the molecular kinematic viscosity, ρ the density and $i = 1, 2, 3$ refers to the x (streamwise), y (spanwise), and z (normal) directions respectively. B_i includes the gravity and the Coriolis force. The dynamic Smagorinsky-Germano subgrid-scale model (Germano et al., 1991) is used.

The dimensions of the computational domain in the streamwise, spanwise and wall-normal directions are, respectively, $l_x = 30H$, $l_y = 6H$ and $l_z = 2H$, H being the boundary layer depth. The grid is uniform in the xy-planes and stretched in the z-direction by a hyperbolic tangent function.

THE MOTION OF SOLID PARTICLES

For particles with a density much greater than the density of the carrier fluid $\left(\rho_p/\rho_f \geq 10^3\right)$, and with a diameter d_p smaller than the Kolmogorov scale, a simplified equation of motion including only the drag and gravity forces can be considered:

$$\begin{aligned} \frac{d\vec{x}_p(t)}{dt} &= \vec{v}_p(t) \ , \\ \frac{d\vec{v}_p(t)}{dt} &= \frac{\vec{v}\left(\vec{x}_p(t),t\right) - \vec{v}_p(t)}{\tau_p} f\left(Re_p\right) + \vec{g} \ , \end{aligned} \tag{2}$$

$\vec{v}_p$ is the velocity of the particle, $\vec{v}\left(\vec{x}_p(t),t\right)$ is the velocity of the fluid at the particle position and $\vec{g}$ is the acceleration of gravity. $\tau_p = \rho_p d_p^2/18\rho_f \nu$ is the particle relaxation time and $Re_p = |\vec{v}_p - \vec{v}|d/\nu$ is the particle Reynolds number. $f\left(Re_p\right) = 1 + 0.15 Re_p^{0.687}$ as proposed by Clift *et al.* (1978). Equation 2 is appropriate for describing the motion of smooth rigid spheres. It neglects the influence of virtual mass and the Basset history force on particle motion.

The driving fluid velocity $\vec{v}\left(\vec{x}_p(t),t\right)$ is given by the velocity field of the LES and a fluctuating subgrid component determined by a modified Lagrangian stochastic model.

STOCHASTIC MODEL FOR THE SUBGRID-SCALE MOTION OF SOLID PARTICLES

Fluid particles

The subgrid-scale velocity of solid particles is given by analogy with the the subgrid-scale stochastic model for fluid particle dispersion, Aguirre et al. (2005). Namely, the Lagrangian velocity of the fluid particle is given by:

$$v_i(t) = \tilde{u}_i(\vec{x}(t)) + v_i'(t) \ . \tag{3}$$

This velocity is considered to have an Eulerian large-scale part $\tilde{u}_i(\vec{x}(t))$ (which is known) and a fluctuating SGS contribution $v_i'(t)$, which is not known and will be modeled by the stochastic approach. The movement of fluid elements at a subgrid level is given by a three-dimensional Langevin model:

$$\left\{ \begin{array}{l} dv_i' = \alpha_{ij}(\vec{x},t) v_j' dt + \beta_{ij}(\vec{x},t) d\eta_j(t) \ , \\ dx_i = v_i dt \ , \end{array} \right. \tag{4}$$

where $d\eta_j$ is the increment of a vector-valued Wiener process with zero mean, $\langle d\eta_j \rangle = 0$, and variance dt, $\langle d\eta_i d\eta_j \rangle = dt\delta_{ij}$. The fluid particle velocity is given by a deterministic part $\alpha_{ij} v_j'$ and by a completely random part $\beta_{ij} d\eta_j$. The coefficients α_{ij} and β_{ij} are determined by relating the subgrid statistical moments of $\vec{v}(t)$ to the filtered Eulerian moments of the fluid velocity, in analogy with van Dop et al. (1986) who developed this approach in the case of a classic Reynolds averaged decomposition. Knowing that the subgrid turbulence is homogeneous and isotropic (basic assumption of the LES), the velocity of fluid elements given by the Langevin model writes as:

$$dv_i' = \left(-\frac{1}{T_L} + \frac{1}{2\tilde{k}} \frac{d\tilde{k}}{dt} \right) v_i' dt + \sqrt{\frac{4\tilde{k}}{3T_L}} \eta_i(t) dt \ . \tag{5}$$

where T_L is the Lagrangian correlation timescale, given by:

$$T_L = \frac{4\tilde{k}}{3C_0\tilde{\varepsilon}} \ , \tag{6}$$

$\tilde{k}$ is the subgrid turbulent kinetic energy, $\tilde{\varepsilon}$ is the subgrid turbulent dissipation rate and C_0 is the Lagrangian constant. The large-scale velocity of the fluid particle is directly computed by the LES with the dynamic Smagorinsky-Germano SGS model. An additional transport equation for $\tilde{k}$ is resolved. This equation is deduced from Deardorff (1980):

$$\frac{\partial \tilde{k}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{k}}{\partial x_j} = \frac{K_m}{3} \frac{g}{\theta_0} \frac{\partial \tilde{\theta}}{\partial z} + 2K_m \tilde{S}_{ij}^2 + 2\frac{\partial}{\partial x_j}\left(K_m \frac{\partial \tilde{k}}{\partial x_j} \right) + \tilde{\varepsilon} \ , \tag{7}$$

where $\tilde{\varepsilon} = C_\varepsilon \tilde{k}^{3/2}/\tilde{\Delta}$. The terms on the right-hand side of equation 7 correspond to the production by buoyancy, the production by shear, the diffusion of $\tilde{k}$ and the dissipation. Since we are interested in neutral flows the potential temperature variation is neglected. The turbulent eddy viscosity K_m is computed by a dynamic procedure as described in the previous section.

Solid particles

Because of its inertia effects and its different responses to gravity, solid particles deviate from the fluid element that originally contained them, inducing a decorrelation. The main difficulty lies in the determination of the fluid particle velocity along the solid particle trajectory, $\vec{v}\left(\vec{x}_p(t),t\right)$. This fluid velocity is computed with equation 3 and by analogy with equation 5 where T_L is replaced by T_L^p, a Lagrangian decorrelation timescale of the fluid velocity along the solid particle trajectory. In order to account for gravity and inertia effects, we expect the modified timescale to be shorter than the fluid Lagrangian timescale T_L. The velocities to which a solid particle is subjected will not be as well correlated as those to which a fluid particles is subjected. Moreover, as noted by Rodgers and Eaton (1990), a frequency measured in a Lagrangian frame is always smaller than a frequency measured in an Eulerian one. Different forms have been previously developed for T_L^p, as Sawford and Guest (1991), Zhuang et al. (1989) for example. We propose the following formulation:

$$T_L^p = \frac{T_L}{\alpha_{grav} + \alpha_{inert}} \ , \tag{8}$$

where α_{grav} and α_{inert} are the coefficients relative to gravity and inertia effects. The gravity effect is estimated following the approximation of Csanady (1963). Csanady proposed an interpolation between the Lagrangian correlation for vanishing inertia and small terminal velocity v_g and the Eulerian correlation for large v_g. In the direction parallel to gravity, with β an empirical constant, α_{grav} is given by:

$$\alpha_{grav} = \sqrt{1 + \left(\frac{\beta v_g}{\tilde{\sigma}} \right)^2} \ , \tag{9}$$

where $\tilde{\sigma} = \sqrt{2\tilde{k}/3}$.

The inertia effect is evaluated in the limit of large inertia and vanishing v_g. A turbulent structure (length scale l), passing by a the moving particle would have a frequency of:

$$\nu_{part} = \frac{|\vec{v}\left(\vec{x}_p(t),t\right) - (\vec{v}_p - \vec{v}_g)|}{\tilde{\sigma}} \nu_L = \alpha_{inert} \nu_L \ . \tag{10}$$

where ν_L represents the Lagrangian correlation timescale.

For the limiting case, when gravity and inertia effects are negligible, the asymptotic behavior is satisfied. Recently, Shao (1995) and Reynolds (2000) have pointed out some contradictions relative to the structure function of $\vec{v}'(\vec{x}_p(t), t)$ and suggested that this velocity should be evaluated using a fractional Langevin equation. In fact, Wiener increments necessarily lead to a structure function proportional to dt when, in the limiting case of large drift velocity and negligible inertia, the driving fluid velocity correlation approaches the Eulerian space-time correlation which is proportional to $dt^{2/3}$. However, the saltating particles being far from these limiting cases, in a way identical to Reynolds (2000), we will forsake considerations of the structure function for increments in fluid velocity and treat $d\eta_j$ as increments of a Wiener process.

PARTICLE COLLISIONS

The developed inter-particle collision model relies on particle pairing and the calculation of the collision probability according to the kinetic theory. This model is inspired by the inter-particle collision model of Sommerfeld (2001), where the generation of a fictious collision partner is replaced by particle pairing.

The domain is divided in boxes that are small compared to the length scale of the flow (Pope, 1985). In each box, at each time step, solid particles are randomly selected by pairs. For each pair (i, j) the probability for the occurrence of a collision is determined. This collision probability is calculated as the product of the time step dt and the collision frequency given by the kinetic theory, Sommerfeld (2001):

$$P_{coll} = f_c dt = \frac{\pi}{4} \left(d_{p,i} + d_{p,j}\right)^2 \left|\vec{v}_{p,i} - \vec{v}_{p,j}\right| n_p dt \; , \qquad (11)$$

where $d_{p,i}$ and $d_{p,j}$ are the particle diameters, $|\vec{v}_{p,i} - \vec{v}_{p,j}|$ is the instantaneous relative velocity of the selected pair and n_p is the number of particles per unit volume in the respective box. In order to decide weather a collision takes place, a random number ξ from a uniform distribution in the interval $[0; 1]$ is generated. A collision occurs when the random number becomes smaller than the collision probability, i.e. if $\xi < P_{coll}$.

The simulated concentration, given by the number of particles obtained by the simulation in each box, and thus dependent on the number of computed trajectories, must be corrected in order to obtain the corresponding actual number of particles per unit volume, n_p, which is used for the prediction of the collision probability. The correction factor depends on the loading ratio and on the total number of simulated trajectories.

The relations of the calculation of the post-collision velocities of the considered particles in the co-ordinate system where one particle is stationary are given by the momentum equations for an oblique central collision. By solving the momentum equations in connection with the Coulomb's law of friction and neglecting particle rotation, one obtains the following equations for the determination of the velocity components of the considered particles after collision, $(v'_{p,i,x}, v'_{p,i,z})$, the symbol prime denoting here the velocity after collision:

$$v'_{p,i,x} = v_{p,i,x} \left(1 - \frac{1+e}{1 + m_{p,i}/m_{p,j}}\right) \; . \qquad (12)$$

For a non-sliding collision:

$$v'_{p,i,z} = v_{p,i,z} \left(1 - \frac{1/7}{1 + m_{p,i}/m_{p,j}}\right) \; . \qquad (13)$$

For a sliding collision:

$$v'_{p,i,z} = v_{p,i,z} \left(1 - \mu(1+e) \frac{v_{p,i,x}}{v_{p,i,z}} \frac{1}{1 + m_{p,i}/m_{p,j}}\right) \; , \qquad (14)$$

where the condition for a non-sliding collision is:

$$\frac{v_{p,i,x}}{v_{p,i,z}} < \frac{7}{2}\mu(1+e) \; . \qquad (15)$$

Here e is the coefficient of restitution, μ is the coefficient of friction, and $m_{p,i}$ and $m_{p,j}$ are the masses of the considered particles. Finally, the velocities of the considered particles are re-transformed in the original co-ordinate system.

TWO-WAY COUPLING

Influence of the presence of particles on the fluid motion has not yet been fully understood. In some cases, e.g. bubble flow, the presence of particles may produce velocity fluctuations of the surrounding fluid whose wavelength is smaller than the particle diameter.

However, it was numerically shown by Pan and Banerjee (1996) that the particles work as if they were an extra burden to the fluid when the particles are small and have much larger density than the surrounding fluid, as is the case in the present study. In such case, the momentum transfer from particles to fluid can be successfully modeled by adding the reaction force against the surface force acting on the particle to the Navier-Stokes equation, equation 1. This model is sometimes referred to as the force coupling model in contrast to the velocity coupling model (Pan and Banerjee, 1996) in which the velocity disturbance around the particle is considered.

When two-way coupling is modeled by the force coupling model, as mentioned above, an extra term appears in the transport equation of the subgrid turbulent kinetic energy, equation 7:

$$\widetilde{u'_k f'_k} = \frac{\rho_p \Phi_p}{\rho_f \tau_p} \left(\widetilde{u'_k u'_k}\left(\vec{x}_p(t), t\right) - \widetilde{u'_k u'_k}\right) \; . \qquad (16)$$

f'_k is the fluctuation component of the force from particles to fluid and ϕ_p is the volume fraction in the grid cell occupied by the particles. Although several formulas have been proposed for the approximation of $\widetilde{u'_k u'_k}(\vec{x}_p(t), t)$, the model by Porahmadi and Humphrey (1983)

$$\widetilde{u'_k u'_k}\left(\vec{x}_p(t), t\right) = \frac{2\tilde{k}}{1 + \tau_p/T_L} \qquad (17)$$

has been adopted for simplicity. Therefore, the additional term in the transport equation of the subgrid turbulent kinetic energy writes as:

$$\widetilde{u'_k f'_k} = -\frac{\rho_p \Phi_p}{\rho_f} \frac{2\tilde{k}}{\tau_p + T_L} \; . \qquad (18)$$

In the case of sand particles in saltation, even very close to the bed the volume fraction Φ_p, is smaller than 10^{-4}. The two-way coupling as well as the inter-particle collisions have a very small influence on the flow dynamics and particle field characteristics.

MODEL PREDICTIONS AND DISCUSSION

Saltating particles over a sand bed, Nalpanis et al. (1993)

A full description of the experimental facility and results can be found in Nalpanis et al. (1993). Here, the main characteristics of the experiment necessary for understanding the simulations are given.

A turbulent boundary layer over a sand bed is generated. Downwind of the vorticity generators the floor is covered with loose sand with a density of $2650kg/m^3$ and with a median diameter of $188\mu m$. The size distribution of the sand particles is log-normal with geometric standard deviations of 1.18. Profiles of mass flux and wind speed are measured at distances $2m$, $4m$ and $6m$ from the upwind edge of the sand bed. Only the measurements made at $6m$ are presented.

The height H of the turbulent boundary layer is 0.2m and the roughness length is $z_0 = 100\mu m$. The mean velocity at the boundary layer edge U_e is $6.3m/s$ and the friction velocity $u_* = 0.35m/s$. Figures 1 and 2 show predicted profiles of mean velocity and turbulent kinetic energy compared to the experimental data. The turbulent kinetic energy profile is compared to the normalized profile measured by Fackrell and Robins (1982), because the corresponding profile was not published by Nalpanis et al. (1993). The mean values are obtained by averaging the fluctuating field over the horizontal extent of the domain and also over a time period sufficiently long to obtain stable statistics. The LES resulted in a fairly accurate prediction of the mean velocity.

For the turbulent kinetic energy the SGS part, the resolved part and the total of the calculated field are separated. The SGS contribution $\tilde{k}$ is obtained from equation 7. The LES shows discrepancies near the wall, where the fluctuations are mostly parameterized. Probably, the increasing anisotropy near the wall is not correctly represented by our correction. In this study, we only consider particles in saltation, which are almost not influenced by the turbulent fluctuations of the flow.

The vertical profile of mean concentration at the end of the saltating bed is shown on figure 3. The computed concentration profile is in good agreement with the experimental results. Even though the turbulence is practically not resolved near the wall, the mean concentration profile of the saltating sand grains is properly simulated. Figure 4 shows the computed time evolution of the mean rise height, compared to the measured mean value. Our results are in good agreement with the experimental results of Nalpanis et al. (1993) as well as with normalized predictions of Owen (1964).

Sand particles in modified saltation, Taniere et al. (1997)

Particles in modified saltation in a turbulent boundary layer over a flat bed are studied in this experiment. Particles with a density of $2500kg/m^3$ and with a median diameter of $60\mu m$, are introduced into the flow by means of an upward moving piston which is driven by an electric motor. Profiles of wind speed, fluid velocity fluctuations, particle velocities and mass flux profiles are measured at the end of the domain.

The height H of the turbulent boundary layer is $0.07m$, the

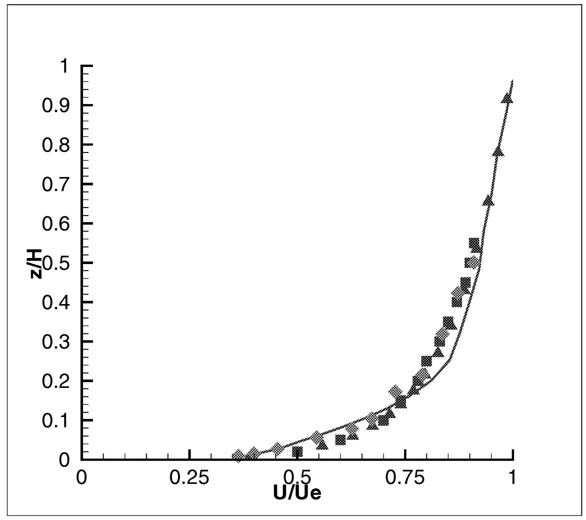

Figure 1: Vertical profile of streamwise mean velocity. Line - LES; Square - FACKRELL & ROBINS (1982); Triangle - log law $u/u_* = 1/klog(z/z_0)$; Diamond - NALPANIS et al. (1993).

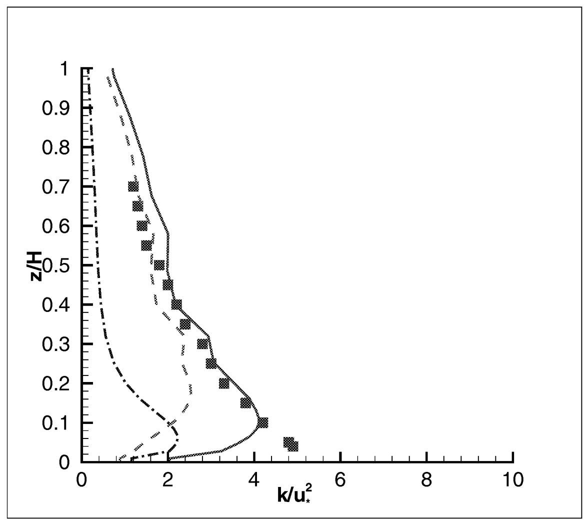

Figure 2: Vertical profile of turbulent kinetic energy. Lines LES: Broken line - resolved; Dashed-dotted - sub-grid; Full line - total; Squares - measurements of Fackrell and Robins (1982).

mean velocity at the boundary layer edge U_e is $10.6m/s$ and the friction velocity $u_* = 0.39m/s$. Figures 5 and 6 show predicted profiles of mean velocity and turbulent kinetic energy compared to the experimental data. The turbulent kinetic energy profile is compared to the normalized profile measured by Fackrell and Robins (1982), because the corresponding profile was not published by Taniere et al. (1997). The LES resulted in a fairly accurate prediction of the mean velocity and of the turbulent kinetic energy (after correction).

The vertical profile of mean concentration at the end of the domain is shown on figure 7. The computed concentration profile is in good agreement with the experimental results. In figure 8, the dimensionless mean velocity profile of the solid phase is displayed and compared with the experimental results on one hand and with the computed fluid velocity profile on

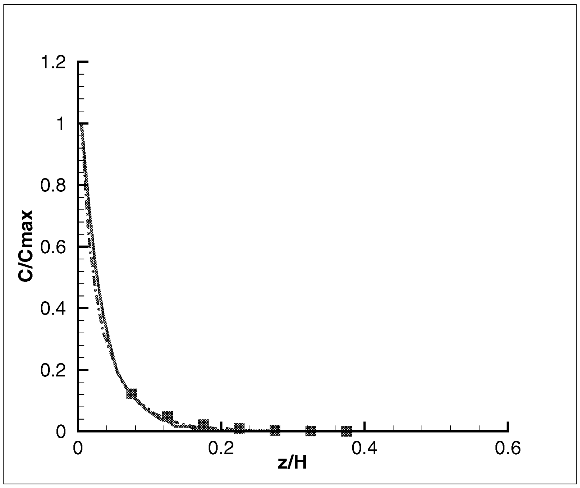

Figure 3: Vertical profile of sand particle concentration at $6m$. Line - LES; Squares - experimental results of Nalpanis et al. (1993).

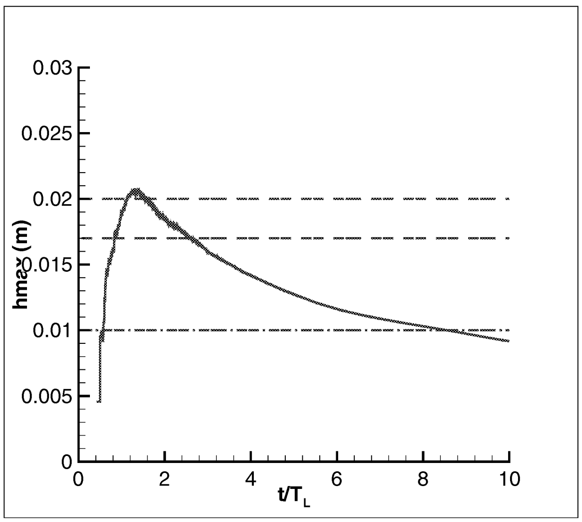

Figure 4: Time evolution of the mean rise height. Line - LES; Dashed-dotted - Nalpanis et al. (1993); Chain - Owen (1964).

the other. The fluid and particle distributions have similar shapes. The computed profiles show good agreement with the experimental results. However, Taniere et al. (1997) found that the mean particle velocity is slightly lower than that of the fluid except very close to the wall. Due to particle-wall interactions the mean velocity of the dispersed phase reaches a nonzero value at the wall.

CONCLUSION

A LES coupled with a Lagrangian stochastic model has been applied to the study of solid particle dispersion in a turbulent boundary layer. Solid particles are tracked in a Lagrangian way. The velocity of the fluid particle along the solid particle trajectory is considered to have a large-scale part and a small-scale part given by a modified three-dimensional Langevin model using the filtered SGS statistics. An appropriate Lagrangian correlation timescale is considered in order to include the influences of gravity and inertia. Two-way coupling and inter-particle collisions are also taken into account. The results of the computations are compared with the wind-tunnel experiments of Nalpanis et al. (1993) and of Taniere et al. (1997). Discrepancies near the lower wall are due to the fact that turbulence in this region is modeled rather than resolved. The LES coupled with the Lagrangian stochastic model provides good description of the dispersion of sand particles in a turbulent boundary layer. Vertical profiles of mean concentration and particle phase velocity match well with the experimental profiles.

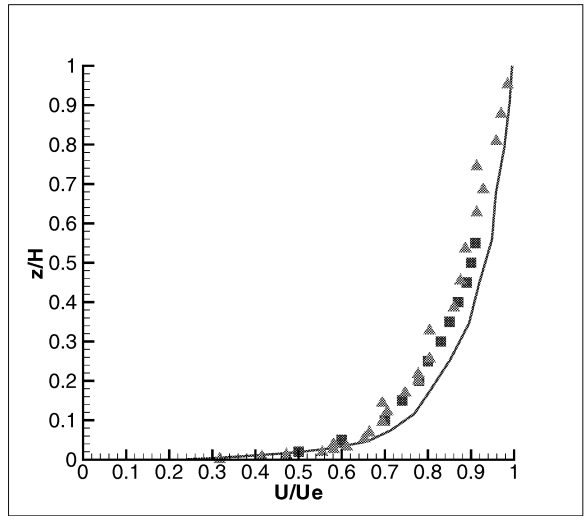

Figure 5: Vertical profile of streamwise mean velocity. Line - LES; Squares - measurements of Fackrell and Robins (1982); Triangle - measurements of Taniere et al. (1997).

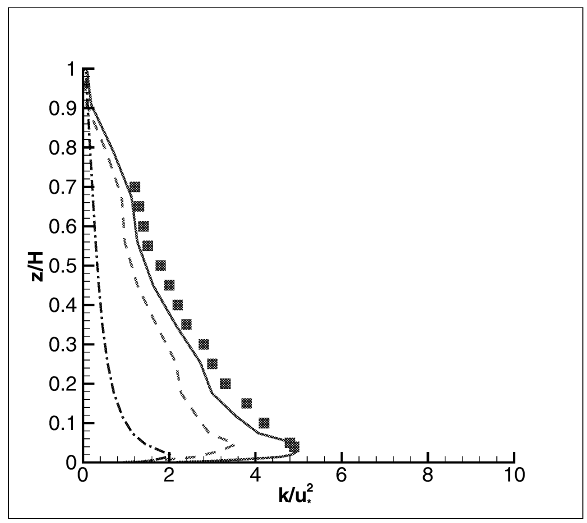

Figure 6: Vertical profile of turbulent kinetic energy. Lines LES: Broken line - resolved; Dashed-dotted - sub-grid; Full line - total; Squares - measurements of Fackrell and Robins (1982).

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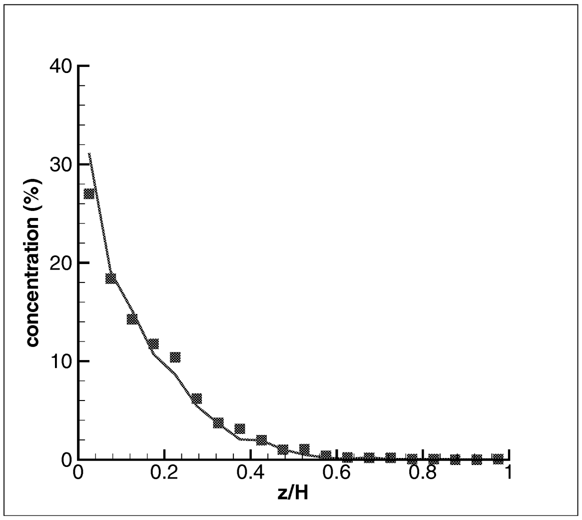

Figure 7: Vertical profile of sand particle concentration at the end of the domain. Line - LES; Squares - experimental results of Taniere et al. (1997).

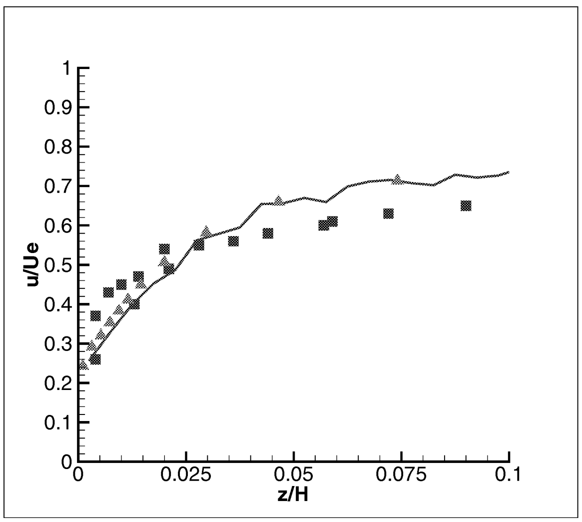

Figure 8: Vertical profile of sand particle mean velocity at the end of the domain. Line - LES for solid particles; Triangles - LES for fluid; Squares - experimental results of Taniere et al. (1997) for solid particles.

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