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Overview of Direct Numerical Simulation of Particle Entrainment in Turbulent Flows

Goodarz Ahmadi*

An overview of removal and re-entrainment of particles in turbulent flows is presented. The procedure for the direct numerical simulation (DNS) of the Navier-Stokes equation via a pseudospectral method for simulating the instantaneous fluid velocity field is described. Particle removal mechanisms in turbulent flows in a duct are examined and effects of the near-wall coherent eddies on the particle detachment and removal are discussed. The particle equation of motion, including the hydrodynamic drag and lift, as well as the Brownian and gravitational forces, are used in the analysis. The simulation results show that large size particles move away roughly perpendicular to the wall due to the action of the shear lift force. Small particles, however, follow the upward flows formed by the near wall eddies in the low speed streak regions. Thus, turbulent near wall eddies play an important role in small particle resuspension, while the lift force is an important factor for re-entrainment of large particles. The results also suggest that small particles primarily move away from the wall in the low speed streaks, while larger particles are mostly removed in the high-speed streaks.

INTRODUCTION

Extensive reviews of the particle adhesion mechanism have been provided by Mittal [1], Corn [2], Krupp [3], Visser [4], Tabor [5], Bowling [6], and Ranade [7]. Accordingly, the van der Waals force makes the major contribution to the particle adhesion force on a surface under dry conditions. The effect of contact deformation on adhesion was first considered by Derjaguin [8]. More recently, Johnson, Kendall, and Roberts [9] used the surface energy and surface deformation effects to develop an improved contact model called the JKR theory. According to this model, at the moment of separation, the contact area does not disappear entirely; instead, a finite contact area exists. Recently, Soltani and Ahmadi ([10], [11]) studied the particle removal mechanisms from smooth and rough walls subject to substrate accelerations.

Extensive reviews on particle removal process from surfaces were provided by Sehmel [12], Nicholson [13], and Smith et al. [14]. Braaten et al. [15] performed an experimental study of particle re-entrainment in turbulent flow. Young et al. [16] reported that the bursting phenomenon has a small effect on entrainment of particles within the viscous sublayer.

A sublayer model for particle resuspension and deposition in turbulent flows was proposed by Cleaver and Yates ([17], [18]). In particular, they suggested that the particle entrainment most likely result from the wall ejection events, while their deposition occurs by the inrush process. A dynamic model for the long-term resuspension of small particles from smooth and rough surfaces in turbulent flow was developed by Reeks et al. [19] and Reeks and Hall [20]. A kinetic model for particle resuspension was proposed by Wen and Kasper [21] and compared with the data from industrial high pure gas systems and with controlled experiments using Latex particles of 0.4-1μm. Wang [22] studied the effect of inceptive motion on particle detachment from surfaces and concluded that the removal of spherical particles is more easily achieved by the rolling motion, rather than sliding or lifting. This result is consistent with the experimental observation of Masironi and Fish [23]. A flow structure-based model for turbulent resuspension was developed by Soltani and Ahmadi ([24, 25]). The DNS simulation was used by Soltani and Ahmadi [26] to study the

*. *Department of Mechanical and Aeronautical Engineering Clarkson University Potsdam, NY, 13699-5725, USA*

particle entrainment process in a turbulent channel flow.

In this work, the particle removal mechanism from a smooth surface in turbulent channel flows is studied. The theories of rolling and sliding detachments are used, and the critical removal condition is analyzed. Effects of various forces and turbulent near wall coherent eddies on turbulent resuspension process are studied. An ensemble of 8192 particles is used in these simulations, and it is shown that turbulence near wall vortical structure and the lift force respectively play important roles in small and large particle re-entrainment and resuspension processes.

TURBULENT FLOW FIELD VELOCITY

The instantaneous fluid velocity field in the channel is evaluated by the direct numerical simulation (DNS) of the Navier-Stokes equation. It is assumed that the fluid is incompressible, and a constant mean pressure gradient in the x-direction is imposed. The corresponding governing equations of motion are:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u} - \frac{1}{\rho^f} \nabla P \tag{2}$$

where $\mathbf{u} = (u_x, u_y, u_z)$ is the fluid velocity vector, P is the pressure, ρ^f is the density, and ν is the kinematic viscosity. The fluid velocity is assumed to satisfy the no-slip boundary conditions at the channel walls. In the simulations, a channel that has a width of 250 wall units, and a 630×630 periodic segment in x and z directions is used. A $16 \times 64 \times 64$ computational grid in the x, y, and z directions is also employed. The grid spacing in the x and z-directions is constant, while the variation of grid points in the y direction is represented by the Chebyshev series. The distance of the i th grid point in the y direction from the centerline is given as

$$y_i = \frac{h}{2} \cos(\pi i / M), \qquad 0 \le i \le M \tag{3}$$

Here h is the channel height, M =64, and there are 65 grid points in the y-direction.

To solve for the velocity components by pseudospectral methods, the fluid velocity is expanded in a three-dimensional Fourier-Chebyshev series. The fluid velocity field in the x and z direction is expanded by Fourier series, while in the y-direction the Chebyshev series is used. The code uses an Adams-Bashforth-Crank-Nickolson (ABCN) scheme to compute the nonlinear and viscous terms in the Navier-Stokes equation and performs three fractional time steps to forward the fluid velocity from time step (N) to time step (N+1). In these computer simulations, wall units are used; and all variables are nondimensionalized in terms of shear velocity u^* and kinematic viscosity ν.

Zhang and Ahmadi [27] showed that the present DNS with a grid size of $16 \times 64 \times 64$ can produce first-order and second-order turbulence statistics that are reasonably accurate when compared with the results of high resolution grids of $32 \times 64 \times 64$ and $32 \times 128 \times 128$. In this paper, for the sake of computational economy, the coarser grid is used.

Figure 1 shows a sample instantaneous velocity field at $t^+ = 100$ in the y-z plane (at $x^+ = 157.5$) perpendicular to the flow directions. While the velocity field has a random pattern, near wall coherent eddies and flow streams towards and away from the wall can be observed from this figure.

ADHESION MODELS

JKR Model

The Hertz contact theory is modified in this model by taking into account the surface energy effects and by allowing for the deformation of particle and substrate surface. Accordingly, a finite contact area forms and the radius of the contact circle, a, is given as

$$a^3 = \frac{d}{2K}\left[P + \frac{3W_A \pi d}{2} + \sqrt{3\pi W_A d P + \left(\frac{3\pi W_A d}{2}\right)^2}\right] \tag{4}$$

where

$$K = \frac{4}{3}\left[\frac{(1-\nu_1^2)}{E_1} + \frac{(1-\nu_2^2)}{E_2}\right]^{-1} \tag{5}$$

is the composite Young's modulus. Here, d is the diameter of the spherical particle, W_A is the thermodynamic work of adhesion, P is the applied normal load, and ν_i and E_i are, respectively, the Poisson ratio and the Young modulus of material i ($i = 1$, or 2).

According to the JKR model, to detach a sphere from a plane surface, the required pull-off force, F_{p_o}, is given by

$$F_{P_o}^{JKR} = \frac{3}{4}\pi W_A d \; . \tag{6}$$

At the moment of separation, the contact radius is finite and is given by

$$a = \frac{a_0}{4^{1/3}} \tag{7}$$

where a_0 is the contact radius at zero applied load given as

$$a_0 = \left(3\pi W_A d^2 / 2K\right)^{1/3} \tag{8}$$

DETACHMENT MODEL

A particle may be detached from a surface when the applied forces overcome the adhesion forces. A

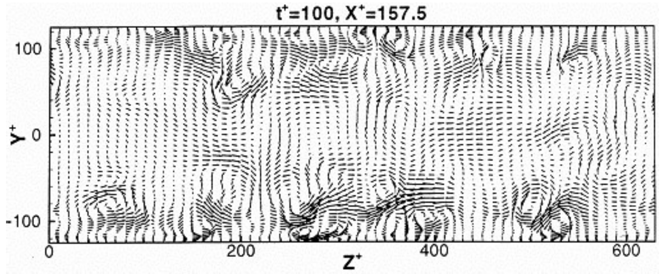

Figure 1. Sample velocity plot in the y-z plane.

particle may lift-off from the surface, slide over it, or roll on the surface. These detachment mechanisms have been discussed by Wang [22]. The moment and sliding detachment mechanisms which are important for particle removal by fluid flows are briefly described here.

Moment Detachment

The critical moment model for the detachment of particles from a surface was studied by Soltani and Ahmadi ([24, 25]). Accordingly, a particle will be detached when the external force moment overcomes the resisting moment due to the adhesion force. That is

$$M_t + F_t\left(\frac{d}{2} - \alpha_0\right) + F_L a \geq F_{P_o} a \tag{9}$$

where F_t is the tangential external force acting on the particle (e.g. the fluid drag force), α_0 is the relative approach between the particle and surface (at equilibrium conditions), M_t is the external moment of the surface stresses about the center of the particle, F_L is the lift force, and F_{P_o} is the particle adhesion force.

Sliding Detachment

Wang [22] studied the effect of inceptive motion on particle detachment. Accordingly, the particle will be removed by sliding if:

$$F_t \geq kF_{P_o}\ . \tag{10}$$

Here F_t is external force (i.e. the fluid drag force) acting on the particle parallel to the surface, and k is the coefficient of static friction.

PARTICLE EQUATION OF MOTION

The equations of motion for a spherical particle moving in a channel flow are given as:

$$\frac{d\mathbf{v}^+}{dt^+} = \mathbf{g}^+ + \mathbf{F}_d^+ + \mathbf{F}_L^+ + \mathbf{n}^+(t^+) \tag{11}$$

and

$$\frac{d\mathbf{x}^+}{dt} = \mathbf{v}^+ \tag{12}$$

where $\mathbf{g}^+$ is the gravity, $\mathbf{F}_d^+$ is the drag force, $\mathbf{F}_L^+$ is the lift force, and $\mathbf{n}^+(t^+)$ is the Brownian random force. (Note that only the y-component of the lift force is considered in this study.) All variables are nondimensionlized by the fluid viscosity, ν and shear velocity, u^*. That is

$$\mathbf{x}^+ = \frac{\mathbf{x}u^*}{\nu},\ \mathbf{v}^+ = \frac{\mathbf{v}}{u^*},\ t^+ = \frac{tu^{*2}}{\nu},$$
$$\mathbf{g}^+ = \frac{\nu}{u^{*3}}\mathbf{g},\ \mathbf{F}_d^+ = \frac{\nu}{u^{*3}}\mathbf{F}_d,\ \mathbf{F}_L^+ = \frac{\nu}{u^{*3}}\mathbf{F}_L \tag{13}$$

Drag Force

For a sphere with no externally applied torque moving in a wall-bounded channel flow, the drag force can be expressed as:

$$\mathbf{F}_d = \frac{6\pi\mu a C_N}{C_c}C^w(\mathbf{u} - \mathbf{v}) \tag{14}$$

where $\mathbf{u} = (u_x, u_y, u_z)$ is the fluid velocity, $\mathbf{v} = (v_x, v_y, v_z)$ is the particle velocity, $a = \frac{d}{2}$ is the particle radius, μ is the coefficient of viscosity, C_i^w is the wall correction factor, and C_c is the Cunningham correction factor given by:

$$C_c = 1 + \frac{2\lambda}{d}\left[1.257 + 0.4\exp\left(-1.1d/2\lambda\right)\right]. \tag{15}$$

Here, λ is the mean free path of the gas.

When the particle Reynolds number based on particle-fluid slip velocity is not small, the drag force deviates from the Stokes expression. The nonlinear correction coefficient to the Stokes drag is given as

$$C_N = 1 + 0.15\,\mathrm{Re}_p^{0.687}\ . \tag{16}$$

Eq. (22 agrees with experiments in the range of $1 < \mathrm{Re}_P < 200$, where Re_p is the Reynolds particle number defined as:

$$\mathrm{Re}_p = \frac{|\mathbf{v} - \mathbf{u}|d}{\nu}\ . \tag{17}$$

Lift Force

The expression for the Saffman lift force for a spherical particle moving in an unbounded shear flow field is given as:

$$\mathbf{F}_L = -\operatorname{sgn}(G) 6.46 \mu a^2 U_s \left[\frac{|G|}{\nu} \right]^{1/2} \vec{\mathbf{y}} \tag{18}$$

where sgn denotes the signum function, $\vec{\mathbf{y}}$ denotes the unit vector in the direction perpendicular to the wall, $U_s = v_x - u_x$ is the particle-fluid slip velocity, and G is the shear rate defined as:

$$G = \frac{du_x}{dy} \ . \tag{19}$$

Hydrodynamic Torque
For a sphere in contact with a plane surface, the hydrodynamic torque acting on the particle is given by

$$M_t = 2\pi \mu C_M d^2 \sqrt{u_x^2 + u_z^2} \tag{20}$$

where $C_M = 0.943993$ is the correction factor for the wall effects.

RESULTS AND DISCUSSION

In this section, particle removal, resuspension and re-entrainment in the turbulent channel flows are studied. A temperature of $T = 298K$, a kinematic viscosity of $\nu = 1.5 \times 10^{-5} m^2/s$, and a density of $\rho^f = 1.12 kg/m^3$ for air, a density ratio of $S = 1964$ for graphite particle, and a shear velocity of $u^* = 1.0 m/s$ are assumed. In this case, the Reynolds number based on the shear velocity,

u^*, and the half-channel width is 125, while the flow Reynolds number based on the hydraulic diameter and the centerline velocity is about 8000. This condition corresponds to a channel width of 3.75mm. To keep the computational effort within an acceptable limit and to reduce the statistical error, ensembles of 8192 (2^{13}) particles for each diameter are used in these simulations. The gravity is assumed to be in the direction perpendicular to the lower wall.

REMOVAL AND ADHESION

In this section, ensembles of different size particles are initially randomly distributed on the lower wall, and all forces acting on each particle are computed at every time step. When the detachment condition (Eqs. (9 or (10)) is satisfied, the particle is assumed to be resuspended in the turbulent flow, and its subsequent motion is simulated using Eqs. (11 and (12).

Particle Detachment Mechanism
In this section, the results for removal of an ensemble of 8192 graphite particles with diameters of $40\mu m$ and $50\mu m$ are described. It is found that all particles detach from the wall by the rolling detachment mechanism. This is consistent with the suggestion of Soltani and Ahmadi [10, 24] that the rolling detachment is the dominant resuspension mechanism of spherical particles in turbulent flows. Hinze [30] summarized the streaky structures of turbulent near wall flows. In the earlier works of Soltani and Ahmadi [24-26] and Zhang and Ahmadi [27], it was shown that the turbulence near wall coherent eddies play a dominant role in particle deposition and resuspension processes. We performed several simulations with ensembles of 8192 particles of different sizes that are initially uniformly distributed on the lower surface of the duct. Figures 2 and 3 shows the locations of particles that remained attached on the lower wall at $t^+ = 40$. For $30\mu m$ particles, Figure 2 shows that the particles are removed in certain bands. The attached particles also form roughly distinct bands. Similar trends are also observed in Figure 3 for $40\mu m$ particles. Here, the structure of bands is more pronounced. In these figure, the distances between the nearby bands are about 100-150 wall units, which is consistent with spacing between high speed and low speed streaks as also was noted by Soltani and Ahmadi [26]. Similar band structures also exist for particles with other diameters. The number of particles that remain attached to the wall, however, decreases rapidly as particle diameter increases. This is because the hydrodynamic forces and torques acting on particles increase faster than the adhesion force as d increases, while the effect of weight is negligible. Figures 2 and 3 further confirm the importance of near flow structure (coherent vortices, high and low

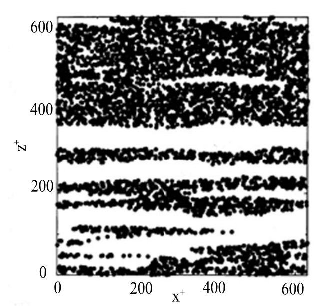

Figure 2. Distribution of the locations of 30 μm particles on the surface.

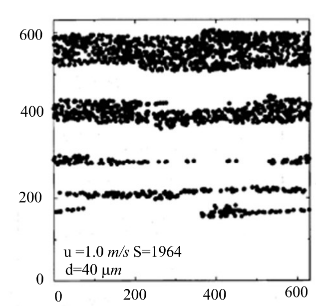

Figure 3. Distribution of the locations of $40\mu m$ particles on the surface.

speed streaks) in particle removal and re-entrainment processes in turbulent flows.

RE-ENTRAINMENT TRAJECTORIES

In this section, ensembles of particle trajectories, which are removed from the wall are computed and statistically analyzed. Here, a particle-to-fluid density ratio of $S = 1964$ and a shear velocity of $u^* = 1.0m/s$ are assumed.

Re-entrainment Process

As noted before, an ensemble of 8192 particles with $d = 40\mu m$ are initially randomly distributed on the lower wall. The particles are assumed to be resuspened when the detachment condition given by Eq. (9 is satisfied. The subsequent trajectories of detached particles are then evaluated using Eq. (11. In this case, $\tau_p = 0.012$ sec and $\tau_p^+ = 780$. Figure 4 shows the instantaneous locations of particles in the y-z plane at time $t^+ = 500$. It is observed that the particle transport away from the wall is not a uniform diffusion process. The periodic spanwise structure can clearly be seen from this figure. The particles seem to move away from the wall on certain distinct bands.

To analyze the re-entrainment process for sub-micrometer particles, the simulation is repeated for an ensemble of 8192 particles with $d = 0.14\mu m$. In this case, $\tau_p = 3.4 \times 10^{-7}$ sec and $\tau_p^+ = 0.023$. The particles are initially randomly distributed at a distance of one wall unit from the lower wall, and their subsequent trajectories are analyzed. Figure 5 shows particle positions in the y-z plane at time $t^+ = 250$. This figure indicates that the 0.14 μm particle concentration in the y-z plane is nonuniform, and the particles tend to move away from the wall in certain bands. These small particles, however, exhibit more dispersion due to the Brownian motion effects.

CONCLUSIONS

Based on the present results, the following conclusions are drawn:

- The rolling detachment is the dominant mechanism for particle removal in turbulent flows.

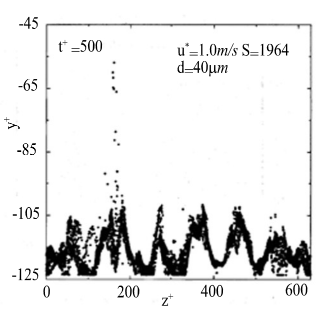

Figure 4. Distribution of 40 μm particles in the$y$ -z plane at $t^+ = 250$.

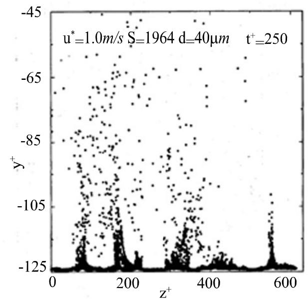

Figure 5. Distribution of 0.14 μm particles in the$y$ -z plane at $t^+ = 250$.

- Drag and hydrodynamic torque are dominant and the effect of lift and gravitational forces on particle detachment from the wall are negligible.
- The turbulence near wall flow structure plays an important role in particle detachment process.
- The instantaneous particle distribution in the y-z plane during the re-entrainment process forms a periodic spanwise structure due to the turbulence near wall coherent eddies.
- The present DNS of turbulent near wall flows further shows that high speed streamwise velocities correspond to those of downward flows (toward the wall), and the low speed streamwise velocity regions correspond to upward flows (away from the wall).
- Turbulence near wall flow structure plays an important role in both large and small particle re-entrainment processes but with different mechanisms.
- Large particles of the order of $d = 40\mu m$ move roughly straight from the wall up to about 10 wall units due to the lift force, and then begin to disperse. These particles move away from the wall faster in the high speed streamwise flow regions.
- Small particles follow the near wall upward flows formed by the coherent near wall vortices in the low speed streamwise velocity regions during their re-entrainment process.

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