Diffusion of nano particles in viscous sub-layer

M. Mahdavimanesh[*1], A. R. Noghrehabadi[2], M. Behbahaninejad[2], G. Ahmadi[3], M. H. Nirooei[1], A. Etminan[1]

[1]Department of Mechanical Engineering, Neyriz Branch, Islamic Azad University, Neyriz, Iran
[2]Department of Mechanical Engineering, Shahid Chamran University of Ahvaz, Neyriz, Iran
[3]Department of Mechanical and Aeronautical Engineering, University of Clarkson, New York, US
mmmahdavimanesh@gmail.com; a.r.noghrehabadi@scu.ac.ir; bnmorteza@scu.ac.ir ;gahmadi@clarkson.edu, m.nirooei@gmail.com, etminan.amin@gmail.com

Abstract: in this paper, diffusion of nano particles from a point source in the viscous sub-layer of turbulent shear flow is considered. the equation of motion of particles including the brownian effects is used and ensembles of 500 particle trajectories are numerically evaluated and statistically analysed. effects of size on particle dispersion and wall deposition processes are studied. the effect of turbulent near a wall is also considered. the results are compared with the exact solution of corresponding eulerian convective diffusion equation in the absence of turbulent fluctuations. the results show that the brownian diffusion play a significant role in the diffusion of nano particles at distances less than 2 wall units from the solid wall.

[M. Mahdavimanesh, A. R. Noghrehabadi, M. Behbahaninejad, G. Ahmadi, M. H. Nirooei, A. Etminan**. Diffusion of nano particles in viscous sub-layer**. *Life Sci J* 2013;10(8s):105-109] (ISSN:1097-8135). http://www.lifesciencesite.com. 13

Keywords: nano particles, viscous sub-layer, Brownian effects, Eulerian convective diffusion equation

Introduction

Analyzing dispersion of small particles suspended in air streams has attracted considerable attention in the past decades. This is because particle diffusion plays a major role in a number of industrial processes such as filtration, separation, particle transport, combustion, air and water pollution, electro photography, microchip, computer manufacturing industries and many others. Small particles suspended in a flowing fluid are simultaneously subjected to Brownian diffusion, turbulent dispersion and gravitational forces. For particle smaller than 5µm Brownian motion has considerable. In particular, near solid surfaces where the intensity of turbulence tends to vanish, Brownian diffusion becomes the dominant transport mechanism.

Diffusion of small particles using the Brownian dynamics (BD) technique was analyzed by Tien, et al. (1977). Simulations of dispersion of sub-micron particles from a point source in uniform and nonuniform flow fields was performed by Saffar-Avval, et al. (2006), O'Brien (1990), Abuzeid, et al. (1991), Li and Ahmadi (1992) and Ounis, et al. (1991).

Deposition of particles on surfaces in turbulent flows had attracted the interest of many researchers. Friedlander and Johnstone (1957) developed the free-flight model for particle deposition process. Liu and Agarwal (1974) analyzed the deposition of aerosol particles in turbulent pipe flows. Wood (1981) and Papavergos and Hedley (1984) and Lain, et al. (2009) summarized the available methods for evaluating the deposition velocity and discussed different mechanism of particle deposition in turbulent flows.

The aim of this work is to simulate diffusion of nano particles from a point source in nonuniform flow near a solid wall. The equation of motion of a solid particle, in addition to the Stokes-Cunningham drag, includes the Brownian force. The Brownian force is modelled as a white noise Gaussian random number process. An ensemble of 500 particle trajectories is considered, wall deposition rate of Brownian particles evaluated and variations of the particle deposition rate with particle size and source location are studied. The results are compared with the exact solution of corresponding Eulerian convective diffusion equation and good agreement is observed.

Equation of motion

The equation of motion of a small particle including the Brownian force is given by (Behzad, et al. (2010), Nasr, et al. (2009)):

$$m\frac{d\upsilon_i^p}{dt}=\frac{3\pi\mu d}{C_c}(\upsilon_i^f-\upsilon_i^p)+mg_i+n_i(t)$$

and

$$\frac{dx_i^p}{dt}=\upsilon_i^p$$

where $m = (\pi/6)\rho^p d^3$ is the particle mass, υ_i is the velocity vector, t is the time, d is the particle diameter, μ is the dynamic viscosity, $n_i(t)$ is the Brownian force, C_c is the Cunningham correction and the superscripts f and p refer to fluid and particle, respectively. For sub-micron particles stocks drag must be corrected by Cunningham factor given as

$$C_c = 1 + \frac{2\lambda}{d}\left[1.257 + 0.4e^{-(1.1d/2\lambda)}\right] \quad (3)$$

where $\lambda = 6.8\times10^{-8}$ is molecular mean free path of carrying fluid.

Using length wall unit υ/u^* and time wall unit υ/u^{*2} the dimensionless form of equation of motion is given by

$$\frac{d\upsilon_i^{+p}}{dt^+} = \frac{1}{\tau_p^+}(\upsilon_i^{+f} - \upsilon_i^{+p}) + n_i^+\left(t^+\right) \quad (4)$$

$$\frac{dx_i^{+p}}{dt^+} = \upsilon_i^{+p} \quad (5)$$

where

$$x_i^+ = \frac{xu^*}{\upsilon}, \qquad v_i^+ = \frac{v_i}{u^*}, \qquad t^+ = \frac{tu^*}{\upsilon} \quad (6)$$

υ is kinematic viscosity, u^* is friction velocity and τ_p^+ is the dimensionless particle relaxation time which is defined as

$$\tau_p^+ = \frac{1}{18}C_c S d^{+2}, \qquad d^+ = \frac{du^*}{\upsilon}, \qquad S = \frac{\rho^p}{\rho^f} \quad (7)$$

where d^+ and S are dimensionless particle diameter and relative density. The dimensionless Brownian force in Eq. (4) is a Gaussian white noise process. The following procedure was used by Li and Ahmadi (1992) and Nasr and Ahmadi (2007)

- Choose a time step Δt
- Generate a sequence of Gaussian random numbers G_i of unit variance zero mean
- Amplitude of the Brownian force that is given by

$$n_i^+\left(t^+\right) = G_i\sqrt{\frac{\pi S_0}{\Delta t^+}} \quad (8)$$

where S_0 is the spectral intensity of the noise as given by

$$S_0 = \frac{648}{\pi C_c^2 ScS^2 d^{+4}} = \frac{2}{\pi Sc\,\tau_p^{+2}}, \qquad Sc = \frac{v}{D} = \frac{3\pi v d\mu}{C_c kT}, \qquad \Delta t^+ = \frac{tu^*}{\upsilon}$$

where Sc is Schmidt number and D is the Brownian diffusivity.

- The entire generated sample of Brownian force need to be shifted by $U\Delta t$, where U is a uniform random number between zero and one.

Figure 1 Shows sample variation of Brownian force for 0.01 μm particle

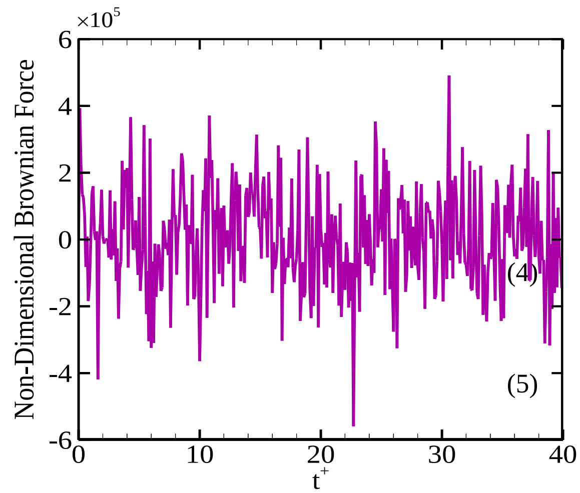

Figure 1: Sample variation of Brownian force for 0.01 μm particle.

Turbulent velocity profile

Mean component of turbulent velocity profile in the viscous sub-layer is given by

$$u^+ = z^+, \qquad \upsilon^+ = 0, \qquad z^+ < 5$$

where z^+ is non-dimensional distance from the wall.

governing eulerin convective diffusion equation

The two dimensional equation of particle concentration released from a point source in nonuniform flow $U_0(z)$ is given by

$$D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right) = \frac{\partial C}{\partial t} + U_0(z)\frac{\partial C}{\partial x} + N_0\delta(x - x_0)\delta(z - z_0)\delta(t - t_0)$$

In this formula N_0 particles are released at time t_0 from the point source of x_0 and z_0 where C and D are particles concentration (particles per unit of volume) and diffusivity, respectively. The variance of particle vertical position is as follow (Li and Ahmadi (1992))

$$\sigma^{+} = \sqrt{2Sc^{-1}t^{+}} \qquad (12)$$

Integrating Eq. (11) over x from $-\infty$ to $+\infty$ yields

$$D\frac{\partial^2 \overline{C}}{\partial z^2} = \frac{\partial \overline{C}}{\partial t} + N_0\delta(z - z_0)\delta(t - t_0), \qquad \overline{C} = \int_{-\infty}^{+\infty} C dx \qquad (13)$$

For $t_0 = 0$ and boundary condition of $\overline{C}\,|_{z=0} = 0$ the total flux at time t to the wall is given by (Ounis, et al. (1991))

$$N_d = \frac{N_0 z_0^{+}}{\sqrt{4\pi t^{+3/2}}} e^{-\left(z_0^{+2} Sc/4t^{+}\right)} \qquad (14)$$

The total number of particles that deposited to the wall during the time interval of $(0-t)$ becomes

$$N_t = \int_0^{t^+} N_d dt^{+} N_0 erfc\left(\sqrt{\frac{z_0^{+2} Sc}{4t^{+}}}\right) \qquad (15)$$

where erfc is the complimentary error function.

Results and discussion

Simulation results for dispersion and deposition of nano particles from a point source are described in this section. Particular attention is given to particle deposition in viscous sub-layer near the solid wall.
A temperature of 298 K, dynamic viscosity of 1.84e-5 kg/s.m and density of 1.225 kg/m^3 for air are used. The friction velocity is 3.7 cm/s. For a density ratio of S = 2000, different particle diameters and various point source distances from the wall are used and particle dispersion is analyzed. Particle trajectories are evaluated by solving Eqs. (4) and (5) using a Rung-Kutta method. The wall boundary condition for particle is sticky wall; it means that as one particle reaches the wall, it sticks to it.
Ensembles of 500 samples are employed and several simulations for various particle diameters between 0.01μm and 0.1 μm are performed.
Figure 2 shows root mean square variation of particle vertical displacement versus time. It is observed that smaller particles disperse much faster than the large ones. This result displays good agreement with exact solution acquired from the corresponding convective diffusion equation.

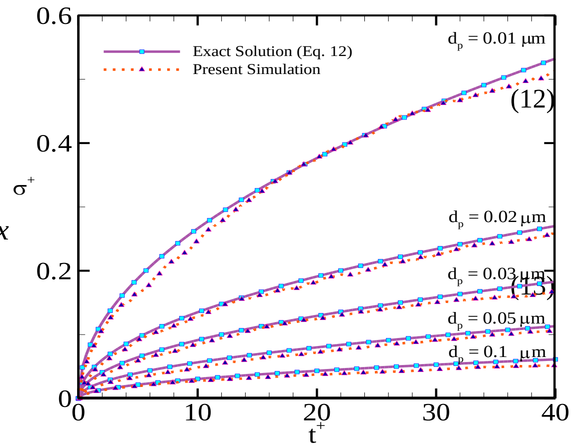

Figure 2. Time variation of RMS vertical particle displacement.

Figure 3 and Figure 4 display variation of deposited particles with time for source distance of 0.5 and 1.0 wall unit. These figures show that number of deposited particles decrease with increase of source distance from the wall. It is also observed that the number of deposited particles increases rapidly as particles diameter decreases.

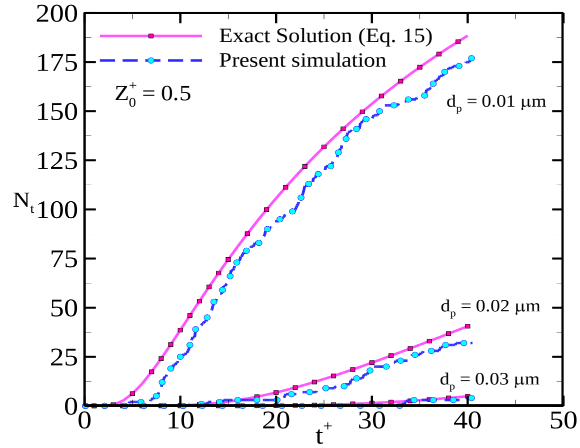

Figure 3. Number of deposited particles with time for different particle diameter and source distance of $z_0^{+} = 0.5$.

Figure 5 shows the variation of the number of deposited particles for different particle size with source distance from the wall. It is observed that increasing source distance from the wall causes particles to deposit less.

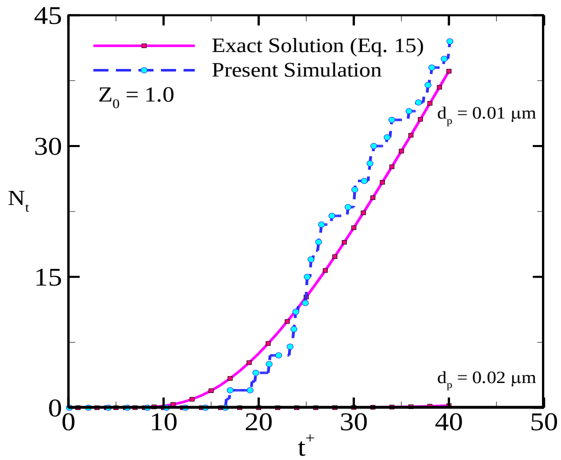

Figure 4. Number of deposited particles with time for different particle diameter and source distance of $z_0^+ = 1.0$.

Figure 6 shows particle statistics including mean, variance and absolute minimum and maximum of trajectory versus time for particles with diameter of 0.01μm and 0.05 μm from a point source at a distance of 1 wall unit. Figure 6a shows that the mean trajectories for 0.01 μm particles move away from the wall as time increases. Figure 6b shows that the mean particle path for 0.05 μm particles remains at about 1 wall unit. It is also observed that Figure 6b has a narrow distribution in the neighbourhood of the point source location while Figure 6a has a wide distribution showing more spreading rate of small particles. The 0.01 μm particles spread about 0.25 wall units due to their significant Brownian motion while the Brownian effect on 0.05 μm particles is less than 0.01 μm particles and therefore their spreading is quite narrow.

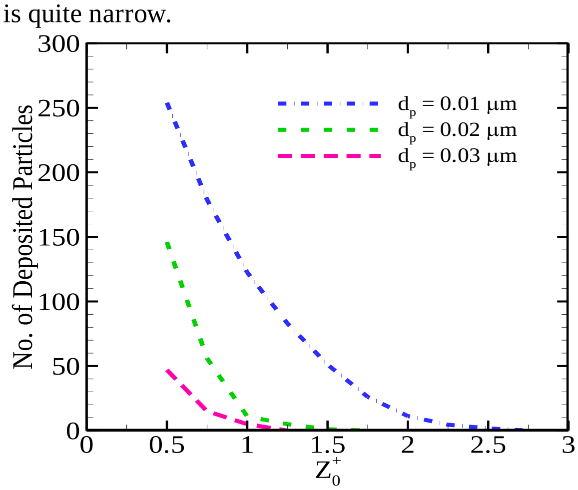

Figure 5. Number of deposited particles with source distance from the wall for different particle diameter and time duration of 100 wall unit.

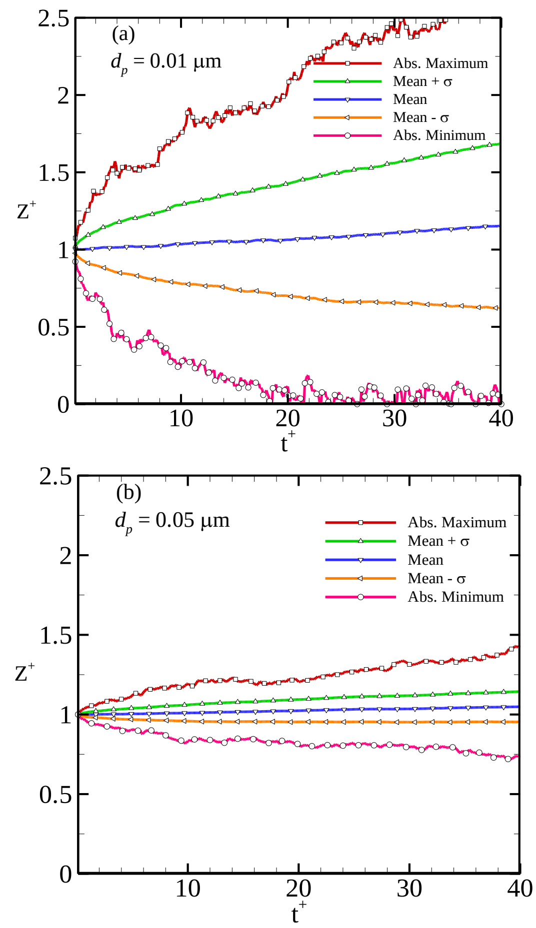

Figure 6. Variation of particle trajectory statics versus time. (a) $d_p = 0.01 \mu m$, (b) $d_p = 0.05 \mu m$.

Conclusion

In this article the dispersion and deposition of nano particles from a point source in a viscous sub-layer are studied. The particle equation of motion, which includes the fluid drag and the Brownian effects, is solved numerically and ensembles of trajectories for particles of different sizes are generated and statistically analyzed. Based on the presented results the following conclusions may be drawn:

- Brownian force significantly affects the inner region of viscous sub-layer of about 1 wall unit from the surface
- Small particle deposition rate increases rapidly with a decrease in particle diameter
- Particle deposition rate increases sharply with reduction of source distance from the wall.

Acknowledgements

This search was supported by the Khuzestan Gas Company.

References

[1] Abuzeid S., Busnaina A. A. and Ahmadi G. (1991). Wall Deposition of Aerosol Particles in a Turbulent Channel Flow. Journal of Aerosol Science, 22, 43-62

[2] Behzad B., Mansoori Z., Saffar-Avval M., Basirat Tabrizi H. and Ahmadi G. (2010). Thermal Stochastic Collision Model in Turbulent Gas–Solid Pipe Flows. International Journal of Heat and Mass Transfer, 53, 1175–1182

[3] Friedlander S. K. and Johnstone H. F. (1957). Deposition of Suspended Particles from Turbulent Gas Streams. Ind. Eng. Chem., 49, 1151-1156

[4] Lain S., Sommerfeld M. and Quintero B. (2009). Numerical Simulation of Secondary Flow in Pneumatic Conveying of Solid Particles in a Horizontal Circular Pipe. Brazilian Journal of Chemical Engineering, 26 583-594

[5] Li A. and Ahmadi G. (1992). Dispersion and Deposition of Spherical Particles from Point Sources in a Turbulent Channel Flow. Aerosol Science and Technology, 16, 209-226

[6] Liu B. Y. H. and Agarwal J. K. (1974). Experimental Observation of Aerosol Deposition in Turbulent Flow. Journal of Aerosol Science, 5,

[7] Nasr H. and Ahmadi G. (2007). The Effect of Two-Way Coupling and Inter-Particle Collisions on Turbulence Modulation in a Vertical Channel Flow. Journal of Heat and Fluid Flow, 28, 1507–1517

[8] Nasr H., G. A. and B. M. J. (2009). A Dns Study of Effects of Particle–Particle Collisions and Two-Way Coupling on Particle Deposition and Phasic Fluctuations. Journal of Fluid Mechanics, 640, 507–536

[9] O'Brien J. A. (1990). Brownian Dynamics Simulation of Very Small Particles: Point Source in Uniform Flow. Journal of Colloid And Interface Science, 134, 497-521

[10] Ounis H., Ahmadi G. and McLaughlin J. B. (1991). Brownian Diffusion of Submicrometer Particles in the Viscous Sublayer. Journal of Colloid And Interface Science, 143, 266-277

[11] Papavergos P. G. and Hedley A. B. (1984). Particle Deposition Behaviour from Turbulent Flows. Chemical Engineering Search, 62, 275-295

[12] Saffar-Avval M., Basirat Tabrizi H., Mansoori Z. and Ramezani P. (2006). Gas–Solid Turbulent Flow and Heat Transfer with Collision Effect in a Vertical Pipe. International Journal of Thermal Sciences, 46, 67–75

[13] Tien C., Wang C. S. and Barot D. T. (1977). Chainlike Formation of Particle Deposits in Fluid Particle Separation. Journal of Science, 196, 983-985

[14] Wood N. B. (1981). Mass Transfer of Particles and Acid Vapour to Cooled Surfaces. Journal of the Institute of Energy, 54, 76-93

4/2/2013