Diffusion of nano particles in viscous sub-layer

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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.

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.


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)): 

\[ m \frac{dv^p}{dt} = \frac{3\pi \mu d}{C_c} (u^f - u^p) + mg_j + n_j(t) \]

and

\[ \frac{dx^p_j}{dt} = u^p_j \]
where \( m = (\pi / 6) \rho^d d^3 \) is the particle mass, \( \mathbf{v}_i \) is the velocity vector, \( t \) is the time, \( d \) is the particle diameter, \( \mu \) 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

\[
C_c = 1 + \frac{2 \lambda}{d} \left[ 1.257 + 0.4e^{-((1.0d/2\lambda))^2} \right]
\]

where \( \lambda = 6.8 \times 10^{-8} \) is molecular mean free path of carrying fluid.

Using length wall unit \( \nu / u^* \) and time wall unit \( \nu / u^*^2 \) the dimensionless form of equation of motion is given by

\[
\begin{align*}
\frac{d\mathbf{v}_i^+}{dt^+} &= \frac{1}{\tau_p^+} (\mathbf{v}_i^+ - \mathbf{v}_i^+ f) + n_i^+(t^+) \\
\frac{dx_i^+}{dt^+} &= \mathbf{v}_i^+
\end{align*}
\]

where

\[
\begin{align*}
x_i^+ &= \frac{x_i}{\nu}, & v_i^+ &= \frac{v_i}{u}, & t^+ &= \frac{tu^*}{\nu}
\end{align*}
\]

is kinematic viscosity, \( u^* \) is friction velocity and \( \tau_p^+ \) is the dimensionless particle relaxation time which is defined as

\[
\tau_p^+ = \frac{1}{18} C_c S d^+ \nu^2, \quad d^+ = \frac{du^*}{\nu}, \quad S = \frac{\rho_p}{\rho^f}
\]

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 \( \Delta t \)
- Generate a sequence of Gaussian random numbers \( G_i \) of unit variance zero mean
- Amplitude of the Brownian force that is given by

\[
n_i^+(t^+) = G_i \sqrt{\frac{\pi S_0}{\Delta t^+}} \]

where \( S_0 \) is the spectral intensity of the noise as given by

\[
S_0 = \frac{648}{\pi C_c Sc^d S d^+} = \frac{2}{\pi \tau_p^+ C_c \mu}, \quad S_c = v^2 D = \frac{3\pi \nu d \mu}{C_c kT}, \quad \Delta t^+ = \frac{tu^*}{\nu}
\]

where \( S_c \) 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 \( \mu \) particle.

**Turbulent velocity profile**

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

\[
\begin{align*}
u^+ &= z^+, & \nu' &= 0, & z^+ < 5
\end{align*}
\]

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

**governing eulerian 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))

$$\sigma^* = \sqrt{2Sc^{-1}}t^*$$

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

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

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))

$$N_d = \frac{N_0 e^{-\frac{z^2}{4Sc}}}{\sqrt{4\pi t} + \frac{3}{2}}$$

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

$$N_t = \int_0^t N_d \, dt \cdot N_0 \operatorname{erfc} \left( \frac{z_0^2 Sc}{4t^*} \right)$$

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.](image)

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 $z_0^* = 0.5$.](image)
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.
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References


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