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A Lagrangian Stochastic Model for Turbulent Dispersion

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A Lagrangian stochastic model is adopted for the calculations of turbulent dispersion in turbulent channel flows. Dispersion of a fluid particle and relative dispersion between two particles released at the same location are investigated and compared with the classical scaling relations for homogeneous turbulence. The viscous effect is realized by adding a Browinian random walk to the calculation of the position of a particle. The near-wall accumulation of particles is examined.

Key Words : Lagrangian Stochastic Model, Brownian Motion, Turbulent Dispersion

1. Introduction

Dispersion of passive contaminant in complex turbulent flows has been extensively studied because of its importance in air pollution or water contamination problems and many industrial applications. However, the mechanism of pollutant dispersion in a turbulent environment is not well understood due to complicated nature of turbulence. In air pollution studies, relatively simple models based on the Gaussian distribution assumption derived from stationary homogeneous flow environment have been used for prediction of particle dispersion. Although such models have been constantly improved for better performance by employing available measured data, application of the model has been limited to simple situations. Epecially particle dispersion in a complex geometry defies such an approach.

Stochastic models were recently proposed to predict turbulent dispersion. Stochastic models have proved to be appropriate for prediction of the dispersion of passive contaminant in high-Reynolds number turbulence. They can take account of unsteadiness, inhomogeneity or non-Gaussianity in the turbulent velocity distribution. Many models were proposed from the meteorology community (Thomson 1987, Flesch and Wilson 1992, Reynolds 1998, Kurbanmuradov and Sabelfeld 2000). They modelled dispersion in the atmospheric boundary layer flow at a very high Reynolds number. Near-wall anisotropy and viscous effect were not taken into account in these models. Even in such a high-Reynolds number atmospheric boundary-layer flow, near-wall modification plays a crucial role in the dispersion of passive contaminant. Furthermore, most models used air pollution problems were derived from the Fokker-Planck equation with the Gaussian probability distribution assumption for distribution of the contaminant. Therefore, the models are not appropriate in an anisotropic situation such as in boundary layer flow or in complex geometry. In the situation that flow is changing in a short time scale, prediction of the flow itself becomes very difficult. Most air pollution models do not solve the flow variables such as velocity and turbulence quantities, instead they assume the flow field. Therefore, these models are applicable only to the cases where the

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flow variables are known *a priori*.

On the other hand, researchers in engineering community have focused on the development of reliable turbulent models for various industrial applications. Recently the Lagrangian probability density function models were adopted for prediction of turbulent reacting flows (Pope 1985, Howarth & Pope 1986, Pope & Chen 1990, Dreeben & Pope 1998). Different terminologies are used in different communities for the same kind of a model; the Lagrangian PDF model and stochastic or random walk model shares the same idea. The Lagrangian PDF model provides a more natural approach than the classical one-point closure model such as $k-\varepsilon$ model. It is able to represent exactly the advection terms which are parameterized in a one-point closure model. Furthermore, Lagrangian models directly provide particle dispersion data, which is one advantage over traditional turbulence models based on an Eulerian average.

The basic approach of Lagrangian models is to treat the trajectory of one particle as one realization among a statistical ensemble of the same flow. In order to obtain the ensemble average, a number of particles are considered simuttareously while two particles can occupy the same place at the same time. The position and velocity of a particle evolve according to the governing equations given in the next section to compute the turbulent velocity field as well as dispersion of fluid elements.

In our previous work (Lee et al. 2000), we introduced a simple Lagrangian pdf model which was applied to a turbulent channel flow at a low Reynolds number. We investigated the performance of the model by comparison with the flow data obtained by direct numerical simulation. In this paper, we will show that the same Lagrangian pdf model can be applied to prediction of particle dispersion. Our model is different from any other particle dispersion models used in most engineering problems. First, our model calculates directly the dispersion of a particle and at the same time the model solves the equations for the flow variables, which will be used in the dispersion calculation. Furthermore, the only assumption in the process of derivation is Kolmogorov's scaling in the inertial region including local isotropy. The model is applicable to nonstationary and anisotropic flow situations. This capability is important when the flow becomes complicated. Second, our model computes dispersion at both the viscous level and the inertial level. Therefore, the model is expected to perform well in a near-wall region as well as in a highly turbulent region. In the previous paper we placed emphasis on the flow variables for evaluation of the model's performance. Here we focus on the dispersion characteristics, in particular, the effects of viscosity and the near-wall behavior of particle dispersion, which have never been reported.

This paper is organized as follows: The governing equations are briefly described in Section 2. The particle dispersion statistics are discussed in Section 3 and we conclude our study in Section 4. The method we adopted for calculation of the probability density distribution for the particle position is explained in the Appendix.

2. Governing Equations

First we describe how the position and velocity of a fluid element evolve in time. In high-Reynolds number turbulence, the dispersion of a passive contaminant follows exactly the same trajectory of the fluid element which carries the pollutant initially. Furthermore, if one considers molecular diffusion as well, the governing equation for the position of a fluid particle can be expressed using the Brownian motion (Einstein 1926),

$$dX_i = U_i dt + \sqrt{2\nu}\, dW_i \tag{1}$$

where X_i, U_i and dt denote the position, the Lagrangian velocity and the time step, respectively. ν denotes molecular viscosity and dW_i denotes the difference of an isotropic Wiener process with a zero mean and the variance dt. The evolution equation for the Lagrangian velocity dU_i can be derived from the Navier-Stokes equation and the Generalized Langevin equation. Refer to Lee et al (2000) for the detailed derivation procedure.

$$dU_i = -\frac{1}{\rho}\frac{\partial\langle P\rangle}{\partial x_i}dt + 2\nu\frac{\partial^2\langle u_i\rangle}{\partial x_j \partial x_j}dt + \sqrt{2\nu}\frac{\partial\langle u_i\rangle}{\partial x_j}dW_j + G_{ij}(U_j - \langle u_j\rangle)\,dt + \sqrt{C_0\langle\varepsilon\rangle}\,dW_i' \quad (2)$$

Here W_i' is another Wiener process independent of W_i. $\partial\langle P\rangle/\partial x_i$, $\langle\varepsilon\rangle$, k and $\langle u_i\rangle$ denote the mean pressure gradient, the turbulent energy dissipation rate, the turbulent kinetic energy and the Eulerian velocity averaged at the position of a particle, respectively. The last term in Eq. (2) is constructed such that scaling in the inertial range is consistent with the Kolmogorov's hypothesis. In the inertial range of the time difference τ, the second order Lagrangian velocity structure function $D_L(\tau)$ $(\equiv\langle(U(t+\tau)-U(t))^2\rangle)$ is proportional to τ with the proportionality constant, C_0. Here $U(t)$ denotes the Lagrangian velocity of a fluid element. The drift coefficient tensor, G_{ij} requires modeling as a function of $\partial\langle u_i\rangle/\partial x_j$, Reynolds stress $\langle u_i' u_j'\rangle$, dissipation $\langle\varepsilon\rangle$. From the condition that the turbulent kinetic energy dissipates at the rate of $\langle\varepsilon\rangle$, the Simple Langevin Model is derived as,

$$G_{ij} = -\left(\frac{1}{2}+\frac{3}{4}C_0\right)\frac{\langle\varepsilon\rangle}{k}\delta_{ij}. \quad (3)$$

This model is a simple model which assumes isotropy. We need a model for the dissipation rate and adopt the following simple representation in this study:

$$\langle\varepsilon\rangle = C_l\frac{k^{\frac{3}{2}}}{l}. \quad (4)$$

Here, l denotes a particular length scale proportional to the mixing length. Using the Van Driest expression for this length scale, one can find

$$l = C_l^{\frac{1}{4}}\kappa y\left(1-\exp\left(-\frac{yu_\tau}{\nu A}\right)\right) \quad (5)$$

where u_τ denotes the wall-shear velocity and can be obtained from:

$$u_\tau = \sqrt{\nu\frac{d\langle u_1\rangle}{dx_2}\bigg|_{wall}}. \quad (6)$$

The coefficients used in this study are, $C_0=2.5$, $C_l=0.09$, $\kappa=0.41$, $A=26$.

3. Results and Discussion

The previous model was applied to the calculation of a turbulent channel flow at $Re_\tau(=u_\tau h/\nu)=100$ and dispersion of particles released at several locations. This flow was chosen so that we could investigate the effect of viscosity and near-wall anisotropy on the dispersion of particles. The flow data for this flow were reported elsewhere (Lee et al. 2000). In this paper, we focus on the dispersion characteristics specially near the solid boundary.

A number of particles are released at the same time at three different wall normal locations and the trajectory of each particle is computed along with the flow data using the model equation in the above. In order to investigate dispersion quantitatively, the statistics of wall-normal and spanwise dispersion are computed. The results of particle dispersion, $\langle(X_i(t+\tau)-X_i(t))^2\rangle$, in the wall-normal and spawise directions are

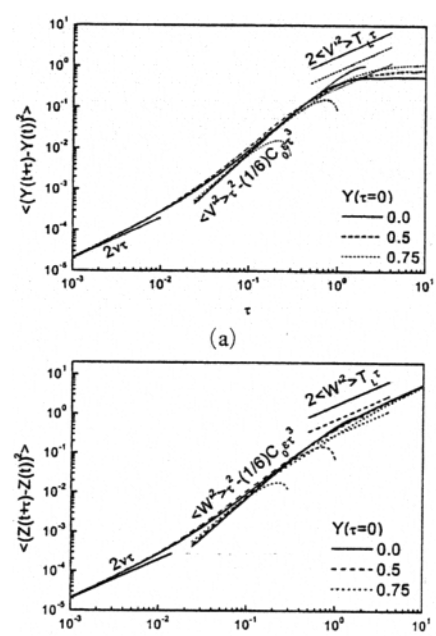


Fig. 1 Dispersion in the wall-normal and spanwise direction of particles released at three different initial locations

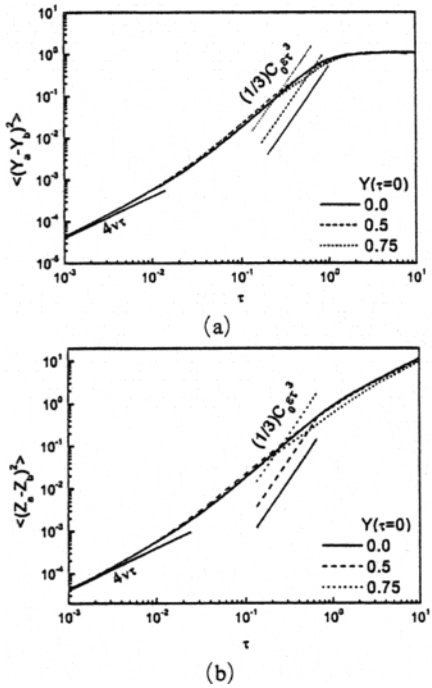


Fig. 2 Relative dispersion between two particles released at the same time in the wall-normal and spanwise direction

shown in Figs. 1 and 2, respectively. The bracket means an ensemble average. Wall-normal dispersion is bounded by the wall while spanwise dispersion occurs linearly with respect to time.

For isotropic turbulence, the scaling expression for dispersion in respective time scales are

$$\langle (X_i(t+\tau) - X_i(t))^2 \rangle = 2\nu\tau \text{ when } \tau \ll \tau_\eta \quad (7)$$

$$= \langle u_i'^2 \rangle \tau^2 \text{ when } \tau_\eta \ll \tau \ll T_L \quad (8)$$

$$= 2\langle u_i'^2 \rangle T_L \, \tau \text{ when } T_L \ll \tau \quad (9)$$

Here τ_η and T_L denote the Kolmogorov time scale and the Lagrangian integral time scale of the velocity correlation, respectively. Equation (7) represents the Brown diffusion and Eqs. (8) and (9) are Taylor's (1921) results for isotropic turbulence. However, Eq. (8) was derived from the assumption that the velocity is perfectly correlated in a short time period. In the inertial range, however, the temporal correlation decays approximately in a linear manner. Consideration of this modifies Eq. (8) as,

$$\langle (X_i(t+\tau) - X_i(t))^2 \rangle = \langle u_i'^2 \rangle \tau^2 - \frac{1}{6} C_0 \varepsilon \tau^3 \quad (10)$$

Examination of Fig. 1 reveals that the inertial range scaling relation is not well confirmed for the two reasons that the inertial range is too narrow due to a low Reynolds number and the deviation term, the second term on the right hand side in Eq. (10), is too small. Furthermore, anisotropy is never considered in the scaling relations.

Such deviation can be investigated by considering of the relative dispersion of two particles released at the same time:

$$f(\tau) \equiv \langle (X_i^a(\tau) - X_i^b(\tau))^2 \rangle \quad (11)$$

where $X_i^a(\tau)$ and $X_i^b(\tau)$ denote the positions of the two particles released at the same location at $\tau=0$. This relative dispersion eliminates the correlated part, the first term in Eq. (10), so that the inertial range scaling can be extracted (Frost & Moulden 1977). Then, $f(\tau)$ becomes,

$$f(\tau) = 4\nu\tau \qquad \text{for } \tau < \tau_\eta \quad (12)$$

$$= \frac{1}{3} C_0 \varepsilon \tau^3 \qquad \text{for } \tau > \tau_\eta \quad (13)$$

Equation (12) is due to the Brown motion. In Fig. 2, the relative dispersions in the wall-normal and spanwise directions are shown. Still, the inertial range scaling with cubic increase is not observed. In the wall-normal direction, the wall boundaries bound growth of the relative dispersion. In the spanwise direction, however, the inertial range is too narrow for such a scaling relation to be valid. In order to confirm such a scaling relation, a higher-Reynolds-number flow should be simulated.

From the relative dispersion the eddy diffusivity, ν_{eddy}, can be defined as,

$$\nu_{eddy} \equiv \frac{1}{2} \frac{d}{dt} \langle (X_i^a(\tau) - X_i^b(\tau))^2 \rangle \quad (14)$$

Corresponding diffusivity in each direction can be easily computed. The scaling relations for isotropic turbulence are

$$\nu_{eddy} = 2\nu \qquad \text{for } \tau \ll \tau_\eta \quad (15)$$

$$= C_0 \varepsilon \tau^2 \qquad \text{for } \tau_\eta \ll \tau \quad (16)$$

which imply that the eddy diffusivity for relative dispersion in the viscous region is twice the molecular viscosity. We also found that the spanwise eddy diffusivity for large time becomes constant. The Richardson's four-thirds law in the inertial range can be written as

$$\nu_{eddy}(r) \sim C\varepsilon^{1/3} r^{4/3} \tag{17}$$

with $r = \langle (X_i^a(\tau) - X_i^b(\tau))^2 \rangle^{1/2}$. To confirm this, we consider the following quantity,

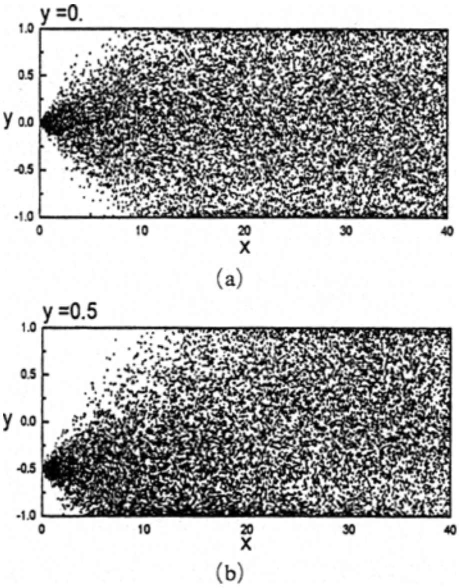


Fig. 3 The eddy diffusivity (a) in the wall-normal and (b) in the spanwise directions

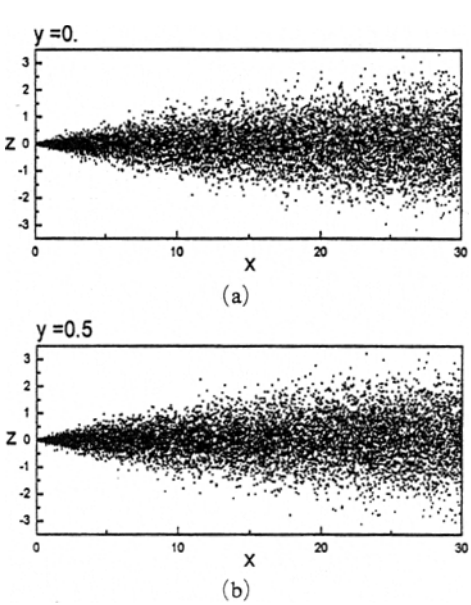


Fig. 4 η of Eq. (18) (a) in the wall-normal and (b) in the spanwise direction

$$\eta = \frac{\nu_{eddy}}{r^{4/3}} \tag{18}$$

In the inertial range, $\eta \sim \varepsilon(constant)$. We found that this trend is not well confirmed in our calculation.

Figures 3 and 4 show the distributions of particles continuously released at a particular location. Two initial release locations, the channel center and the near-wall location are considered. Early dispersion is dependent on the release position. However as time increases, the distribution in the wall normal direction seems to

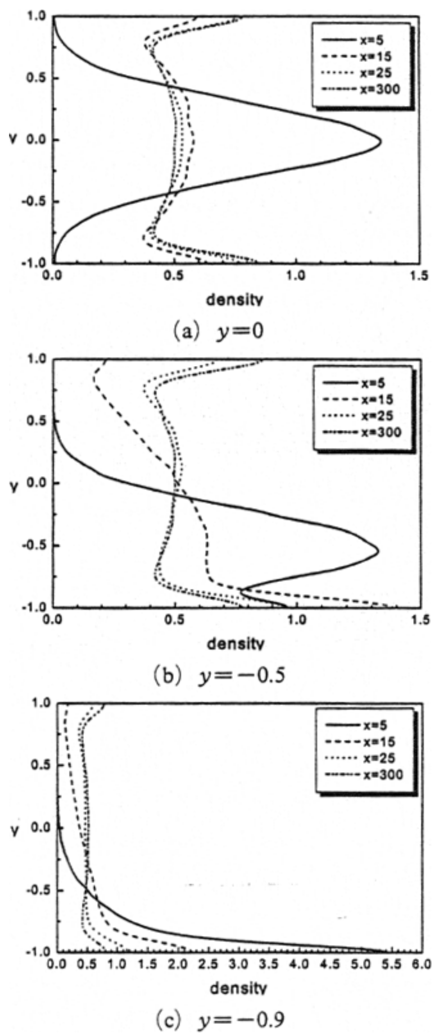
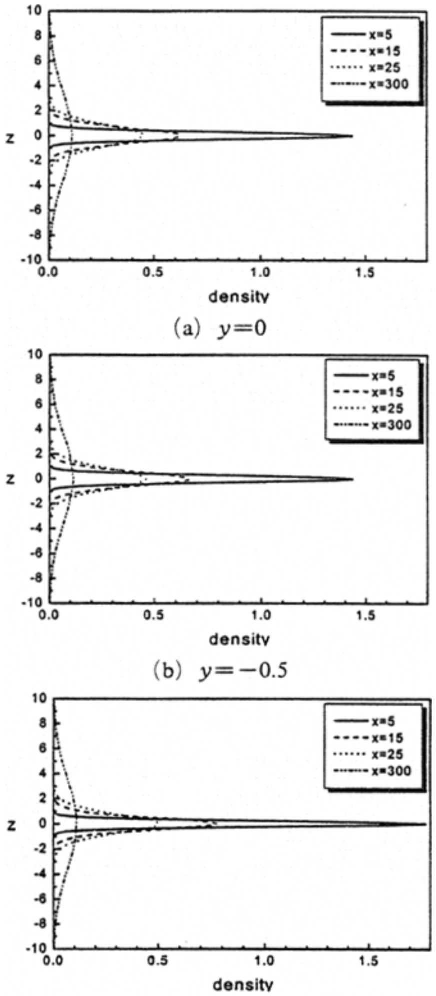


Fig. 5 Distribution of particles in the x-y plane continuously released at: (a) Y(0) =0; (b) Y(0) = −0.5



(a) $y=0$

(b) $y=-0.5$

(c) $y=-0.9$

Fig. 6 Distribution of particles in the x-z plane continuously released at: (a) Y(0) =0; (b) Y (0) = −0.5

approach a fixed distribution profile regardless of the release location. It should be noted that the converged distribution is not uniform across the channel. Particles appear to accumulate near the wall. This can be more pronounced in the distribution of the probability density of the particle's expected position at several downstream locations as shown in Figs. 5 and 6. The probability density distribution from an ensemble of particle's position data is obtained using the method of Silverman (1993). Details may be found in the Appendix. It is clearly shown that the peak den-

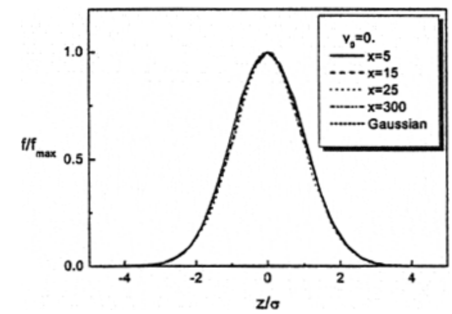


Fig. 7 Probability density distribution in the wall-normal direction at several downstream locations for the position of particles released at three different wall-normal locations: (a) y=0. (channel center); (b) y=0.5 (half way from the wall; (c) y=0.9 (10 % of half channel gap from the wall)

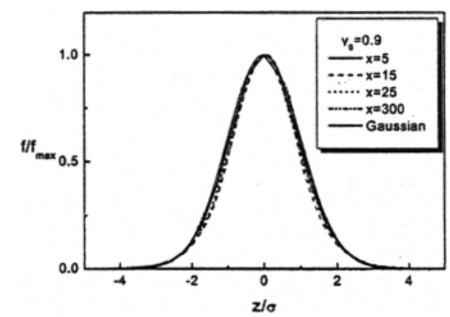


Fig. 8 Probability density distribution of particle's position in the spanwise direction at several downstream locations

sity is found at the wall with the magnitude of about twice the magnitude at the center. The minimum density is observed near the wall, around at $y^+=25$, implying that particles are trapped in the region between the wall and $y^+=25$. Near the wall, turbulence is relatively suppressed although a significant amount of turbulence production occurs there. Also, the dissipation has the peak at the wall. Turbulent dispersion is prohibited by the presence of the wall. The mean flow is slow in that region. Therefore, once a particle dispersed into the near-wall region from the outer region, it has a less chance to leave the near-wall region where dispersion is only due to viscosity at a much slower time scale than turbulent dispersion.

On the other hand, dispersion in the spanwise direction is hardly influenced by the wall as shown in Fig. 6. The spanwise dispersion normalized by the standard deviation at the respective time is shown for two initial release positions in Figs. 7 and 8. In most locations, the distribution is well approximated by the normal distribution.

4. Conclusion

A simple Lagrangian stochastic model derived from the Simple Langevn Model is applied to the computation of dispersion in a turbulent channel flow. Dispersion at the viscous level is simulated by using the Brownian motion of fluid elements. Dispersions at both the viscous time scale and the inertial range are calculated through an ensemble of particle trajectories starting at the same position in the channel. Initial dispersion characteristics are dependent on the release location, but far-downstream distribution of the particles shows almost the same nonuniform distribution. Particles tend to be trapped in the near-wall region mainly in $y^+ < 25$. Such accumulation in the near-wall region was reported in other kinds of flow (Choi & Lee 2001). Scaling relations of dispersion are compared against the classical scaling relations for homogeneous turbulence. The scaling relation in the viscous range is correctly simulated, which the inertial range scaling is partially predicted due to the narrow inertial range. Also, from the turbulence modeling point of view, the current model is not complete in that the simplest model for dissipation is chosen and the dissipation rate models main dispersion due to turbulence.

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References

Dreeben, T. D. and Pope, S. B. , 1998, "Probability Density Function/Monte Carlo Simulation of Near-Wall Turbulent flows," *Journal of Fluid Mechanics*, Vol. 357, pp. 141~166.

Choi, J. and Lee, C., 2001, "Numerical Study of Shear-Enhanced Turbulent Diffusion," *Trans. KSME B* Vol. 25, pp. 944~951.

Einstein, A., 1926, *Investigations on the Theory of the Brownian Movement.*

Flesch, T. K. and Wilson, J. D., 1992, "A Two-Dimensional Trajectory-Simulation Model for Non-Gaussian, Inhomogeneous Turbulence Within Plant Canopies," *Boundary-Layer Meteorology*, Vol. 61, pp. 349~374.

Frost, W., and Moulden, T. H., 1977, *Handbook of Turbulence.*

Howarth, D. C. and Pope, S. B., 1986, "A PDF Modeling Study Self-Similar Turbulent Shear Flows," *Physics of Fluids*, Vol. 30, No. 4, pp. 1026~1044.

Kurbanmuradov, O. and Sabelfeld, K., 2000, "Lagrangian Stochastic Models for Turbulent Dispersion in The Atmospheric Boundary Layer," *Boundary-Layer Meteorology*, Vol. 97, pp. 191~218.

Lee, C., Kim, B. and Kim, N. 2000, "A Simple Lagrangian Pdf Model for Wall-Bounded Turbulence," *KSME International Journal*, Vol. 14, pp. 900~911.

Pope, S. B. 1985, "Pdf Methods for Turbulent Reactive Flows," *Progress in Energy and Combustion Sciences*, 11, pp. 119~192.

Pope, S. B. and Chen, Y. L., 1990, "The Velocity-Dissipation Probability Density Function Model for Turbulent Flows," *Physics of Fluids A*, Vol. 2, No. 8, pp. 1437~1449.

Reynolds, A. M., 1998, "On Trajectory Curvature as a Selection Criterion for Valid Lagrangian Stochastic Dispersion Models," *Boundary-Layer Meteorology*, Vol. 88, pp. 77~86.

Silverman, B. W., 1993, *Density Estimation for Statistics and Data Analysis.*

Taylor, G. I., 1921, "Diffusion by Continuous Movements," *Proc. London Math. Soc., 20, pp. 196~212.*

Thomson, D. J., 1987, "Criteria for the Selection of Stochastic Models of Particle Trajectories in Turbulent Flows," Journal of Fluid Mechanics, Vol. 180, pp. 529~556.

Appendix

Kernel estimation of probability density

A weight function satisfying the following condition is chosen first.

$$\int_{-\infty}^{+\infty} w(x, y)\, dy = 1 \tag{19}$$

$w(x, y) \geq 0$ for all x, y

Then using w which is decaying symmetrically around x, for a given discrete data, X_i, $i=1, \cdots, n$ a probability density distribution can be estimated as:

$$\hat{f}(t) = \frac{1}{n}\sum_{i=1}^{n} w(X_i, t) \tag{20}$$

which also satisfies Eq. (19). The smoothness of $\hat{f}$ depends on $w(x, \cdot)$. If using the kernel estimate for the weight function,

$$w(x, y) = \frac{1}{h}K\left(\frac{y-x}{h}\right). \tag{21}$$

In the near-wall region, the mirror image of the weight function is used for impermeability:

$$w(x, y) = \frac{1}{h}K\left(\frac{y-x}{h}\right) + \frac{1}{h}K\left(\frac{y+x}{h}\right) \tag{22}$$

for x, $y>0$ (boundary at $y=0$)

We chose the following Gaussian distribution for the kernel function:

$$K(t) = \frac{1}{\sqrt{2\pi}} e^{\frac{1}{2}t^2} \tag{23}$$

The optimum value of the kernel width, h, is obtained from the following criterion (Silverman, 1993):

$$h_{opt} = \left(\frac{4}{3}\right)^{1/5} \sigma n^{-1/5} = 1.06\sigma n^{-1/5} \tag{24}$$

where σ denotes the standard deviation of the distributed data.