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Analysis of tracer particle migration in inhomogeneous turbulence

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Abstract

Previous studies [J.M. Maclnnes, F.V. Bracco, Stochastic particle dispersion modeling and the tracer particle limit, Physics of Fluids A 4 (1992) 2809–2824; X.Q. Chen, Heavy particle dispersion in inhomogeneous, anisotropic, turbulence flows, International Journal of Multiphase Flow 26 (2000) 635–661; T.L. Bocksell, E. Loth, Random walk models for particle diffusion in free-shear flows, AIAA Journal 29 (2001) 1086–1096] have shown that the commonly applied stochastic separated flow (SSF) model predicts unphysical results when dealing with the dispersion of tracer particles in inhomogeneous flows. This problem is explored, with regards to the discontinuous random walk model, by considering an idealized flow with constant mean velocity with two regions of constant turbulent kinetic energy. Using the probability density functions (PDFs) for the turbulent velocities it is shown that there is a higher probability of particles traveling into the low kinetic energy region than there are traveling to the region of high kinetic energy, thus resulting in a net migration of particles to the region of low kinetic energy. Corrections that apply a correction velocity and/or adjust the fluctuating velocity based on the local value of the turbulent kinetic energy are analyzed and tested.

Keywords: Tracer particles; Inhomogeneous turbulence; Unphysical migration

1. Introduction

Many engineering applications involve the motion of particles in turbulent flows. For example, the behavior of liquid fuel droplets plays an important role in determining the combustion characteristics and efficiency of gas turbines, diesel engines and spray combustion systems. In addition, due to environmental concerns, the dispersion of pollutants in the atmosphere from industrial plants needs to be monitored. There is thus a need for mathematical models that predict particle motion in turbulent flows.

The stochastic separated flow (SSF) approach is a class of models that is commonly applied to solve engineering problems. This method tracks trajectories of individual particles with the turbulence treated stochastically. Previous research has demonstrated, however, that these models predict unphysical results for the case of very small tracer particles in the presence of inhomogeneous turbulence. These models can produce an unphysical migration of particles resulting from the inhomogeneity.

2. Background

The stochastic differential equation (SDE) model, that manipulates the particle equation of motion into a stochastic differential equation called the Langevin equation, is typically applied to the dispersion of tracer particles in the atmosphere. In 1981, Wilson et al. [4] found that his Markovian chain model, derived from the Langevin equation, predicted an unphysical migration of tracer particles in inhomogeneous turbulence. By comparing the flux densities for homogeneous and inhomogeneous turbulence, it was concluded that a bias needed to be added to the fluctuating velocity to counteract the mean drift. Legg and Raupach [5] later derived a very similar bias by arguing that a force should be added to the Langevin equation due to the mean pressure gradient that accompanied a gradient in the fluctuating turbulent velocity. Thomson [6]

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Nomenclature

A	cross-sectional area, m^2
C	particle concentration, (# particles/volume)
C_D	drag coefficient
C_μ	dimensionless constant with a value of 0.09
d	diameter, m
f	ratio of drag coefficient to Stokes drag $(1+0.15Re_p^{0.687})$
$f(\cdot)$	probability density function
g	acceleration due to gravity, m/s^2
k	kinetic energy, m^2/s^2
l_e	eddy length scale, m
m	mass, kg
n	number of sub-time steps
N	total number of particles injected into the flow
ΔN_i	number of particles in control volume i
$P(\cdot)$	probability
Re_p	particle Reynolds number $(\rho_f d_p \lvert\vec{u}_f - \vec{u}_p\rvert/\mu)$
t	time, s
t_e	eddy lifetime, s
Δt	time step, s
Δt_{sub}	sub-time step, s
u	instantaneous velocity in the x-direction, m/s
U	mean velocity in the x-direction, m/s
v	instantaneous velocity in the y-direction, m/s
V	mean velocity in the y-direction, m/s
v'_c	correction velocity in the y-direction, m/s
$v'_{c,sub}$	correction velocity in the y-direction applied at every sub-time step, m/s
x, y	Cartesian coordinates, m
Δy_i	y-dimension of control volume i, m

Greek symbols

Γ	random variable
ε	dissipation rate, m^2/s^3
μ	molecular dynamic viscosity, kg/m/s
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3
σ^2	variance of fluctuating velocity $((2/3)k)$
τ_p	particle relaxation time, s

Subscripts

$(\cdot)_f$	property of the fluid
$(\cdot)_p$	property of the particle

Superscripts

$(\cdot)'$	fluctuating component
$\overline{(\cdot)}$	time averaged component

took a different approach. He found that it was the way in which the fluctuating component of the turbulence velocity was being randomized that caused the problem. His correction involved modifying the random component of the velocity by using non-Gaussian forcing terms. This method was later extended by Iliopoloulos and Hanratty [7] and Mito and Hanratty [8].

Sawford [9] and Thomson [10] introduced a well mixed condition that stochastic models should abide by in order to obey the second law of thermodynamics. The well-mixed condition basically states that an initially uniform distribution of tracer particles be maintained. Pope [11] found that in order to satisfy this condition the calculated mean velocity field needs to satisfy the continuity equation thereby requiring the proper incorporation of the mean pressure gradient into the dispersion model.

In 1992, MacInnes and Bracco [1] found that random walk models (both continuous and discontinuous) also predict an unphysical migration of tracer particles in inhomogeneous turbulence. Random walk models decompose the instantaneous turbulent velocity that is required for the particle equation of motion into two components: a mean velocity that is found from a turbulence model and a fluctuating velocity, which is modeled as a discontinuous or continuous random function. For the discontinuous random walk model, MacInnes and Bracco proposed normalizing the fluctuating velocity by multiplying it by the local (or updated) turbulence intensity via the kinetic energy at sub-time steps as well as adding a bias to the mean turbulence velocity. The bias found from MacInnes and Bracco took the same form as the Wilson et al. [4] correction, derived for the SDE model, except for an empirical constant. Chen [2] proposed continuously normalizing the fluctuating velocity with the local turbulence intensity found from a second-moment closure model. Bocksell and Loth [3] derived a bias that was very similar to that of MacInnes and Bracco but they applied it to the sub-time step level. Details of the derivation of the bias velocities for the discontinuous random walk models will be provided in a later section.

The current research analyzes the effectiveness of normalizing the fluctuating velocity with the local (or updated) turbulence intensity and shows that updating the kinetic energy to the local value is not sufficient to remove the false migration. Further, it is shown that that method can be equivalent to applying a velocity correction to the particle trajectory calculation. Finally, the existing velocity corrections [1,3] as well as a new one that was developed by the authors are compared.

3. Particle dispersion model

SSF models use a Lagrangian framework to solve for the trajectory of each particle. The Lagrangian particle equation of motion proposed by Basset [12], Boussinesq [13] and Oseen [14] and later extended by Tchen [15] is most often used. For real particles that have a much greater density than the fluid, the particle equation of motion reduces to

$$\frac{d\vec{u}_p}{dt} = \frac{f}{\tau_p}(\vec{u}_f - \vec{u}_p) + \vec{g}, \tag{1}$$

where τ_p is the particle time constant for Stokes flow,

$$\tau_p = \frac{\rho_p d_p^2}{18\mu}, \tag{2}$$

f is the ratio of the drag coefficient to Stokes drag,

$$f = 1 + 0.15Re_p^{0.687}, \tag{3}$$

and Re_p is the particle Reynolds number,

$$Re_p = \frac{\rho_f d_p|\vec{u}_f - \vec{u}_p|}{\mu}. \tag{4}$$

The discontinuous random walk model (otherwise known as the discrete eddy model) assumes the particles interact with a series of discrete turbulent eddies. Every time a particle enters a new eddy, it is exposed to a new instantaneous velocity, which is held constant for the duration of the particle/eddy interaction time. The instantaneous turbulent velocity field can be decomposed into a mean velocity and a random fluctuating velocity. The isotropic Shuen, Chen and Faeth [16] model determines the fluctuating velocity by

$$\vec{u}_f'(t) = \vec{\Gamma}\sqrt{\tfrac{2}{3}k}, \tag{5}$$

where Γ is a random variable sampled using a Gaussian distribution of zero mean and unity variance.

The duration that a particle remains exposed to each eddy or instantaneous velocity is determined from the eddy interaction time. The eddy interaction time is calculated to be the minimum of the eddy lifetime and the time for a particle to cross an eddy. Lighter particles have a tendency to follow the fluid particle and will remain within the eddy for the duration of the eddy's lifetime. The Shuen, Chen and Faeth [16] model expresses the eddy lifetime as

$$t_e = \frac{l_e}{(\frac{2}{3}k)^{1/2}}, \tag{6}$$

where l_e is the dissipation length scale which is defined as

$$l_e = C_\mu^{0.75}\frac{k^{3/2}}{\varepsilon}. \tag{7}$$

C_μ is a turbulence model constant with a value of 0.09. Tracer particles represent the limit where the particles time constant, τ_p, is small relative to the smallest turbulence scales.

4. Unphysical predictions for tracer particles

Discontinuous random walk models predict unphysical results when dealing with the dispersion of tracer particles in inhomogeneous flows. This statement can be easily proven by reducing the dispersion problem to a case where the fluid motion is divergence free and the particles follow the same path as the fluid particles, i.e., tracer particles. When a uniform concentration of particles is injected along the entire inlet region of a system, the same uniform concentration should remain throughout the system, regardless of the inhomogeneity of the turbulence (in the same way that an isothermal flow would remain isothermal irrespective of the turbulence). It can be shown, however, that the models predict an unphysical migration of particles from the region of high turbulence intensity to the region of low turbulence intensity.

To demonstrate that the Shuen, Chen and Faeth [16] model predicts unphysical particle migrations in inhomogeneous turbulence, two idealized inhomogeneous cases are simulated. All cases use a uniform mean flow with particles released uniformly from the inlet.

4.1. Case 1 – Kinetic energy step function

The first test case involves a kinetic energy step function. The ratio of the kinetic energy to the dissipation rate is kept constant throughout the domain. This will ensure a uniform eddy lifetime and therefore a uniform time step (for the case of tracer particles). A summary of the flow properties are as follows:

$$U = 5\ \text{m/s}, \quad V = 0\ \text{m/s}, \quad \frac{k}{\varepsilon} = 1.491\ \text{s},$$

$$k = \begin{Bmatrix} 0.1\ \text{m}^2/\text{s}^2 \to y < 0\ \text{m} \\ 0.5\ \text{m}^2/\text{s}^2 \to y > 0\ \text{m} \end{Bmatrix}.$$

A uniform grid is used as shown in Fig. 1. A total of 12 million tracer particles are injected uniformly along the entire inlet region (which was found to be statistically significant). By defining $U \gg \sqrt{\overline{u'^2}}$ the x-dimension (axial direction) of the control volumes can be chosen to be the distance a particle travels during a time step. Thus, particles travel a full control volume during each time step, which eliminates dispersion in the axial direction. Since tracer particles that follow the fluid flow exactly are considered, the particle velocity is set to the sampled gas phase velocity.

Normalized particle concentration profiles are calculated for several downstream locations. The particle concentration profiles are normalized by the particle concentration at the inlet. If there were no net particle migration, the normalized particle concentration profiles would be uniform and equal to unity at all downstream locations. Fig. 2 shows the predicted particle concentration after 1, 5, and 9 eddy lifetimes. From the figure, it is clear that the Shuen, Chen and Faeth [16] model predicts a clear migration of particles from the region of high turbulent intensity to low turbulent intensity. This particle migration is amplified downstream from the inlet.

The particle migration occurs because a greater number of particles are moving towards regions of low turbulence intensity than there are moving to regions of high turbulence intensity. This is because particles from regions of

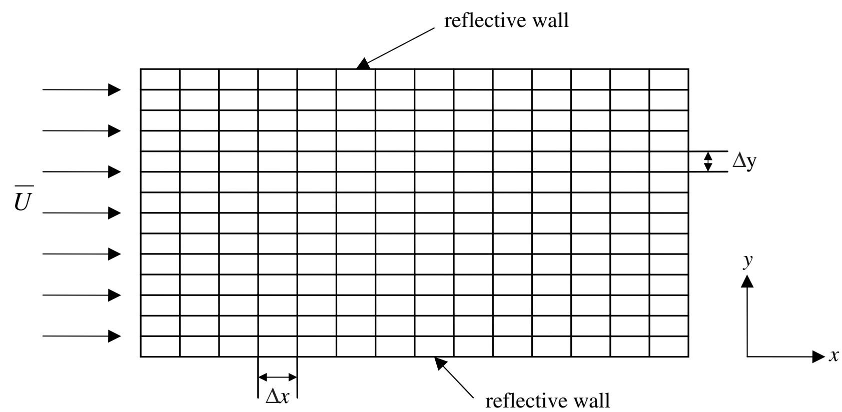

Fig. 1. Grid domain used in test cases.

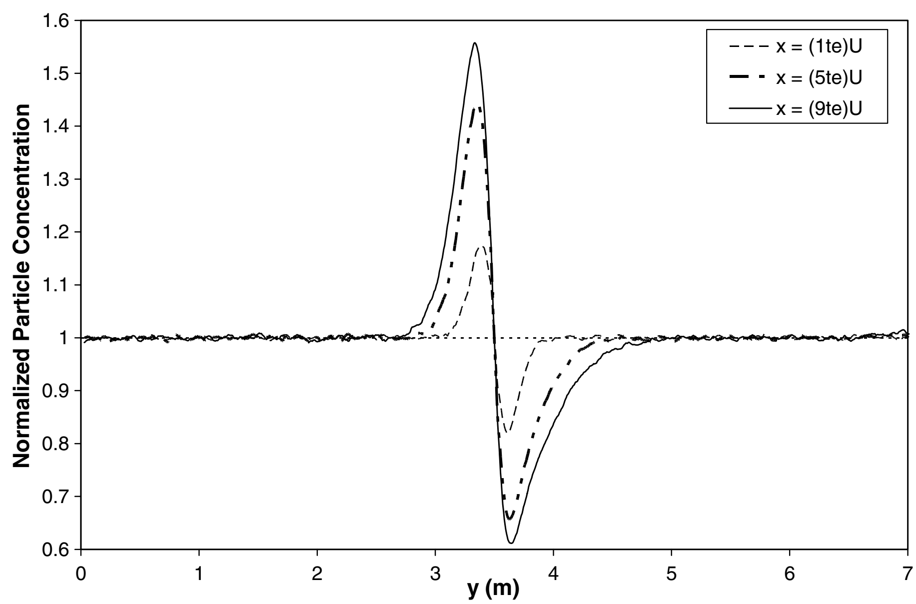

Fig. 2. Normalized particle concentration profiles for first test case at different locations downstream from the inlet.

high turbulence intensity on average can travel a greater distance than particles from a lower turbulence intensity region during the same time interval [1]. Thus the high velocity particles from the high kinetic energy region are able to penetrate into the low kinetic energy region, yielding a non-uniform particle concentration. This can be illustrated mathematically since the probability density functions (PDFs) for the turbulent velocities can be used to determine the probability of particles to travel into each turbulent kinetic energy region. As in the Shuen, Chen and Faeth [16] model, the PDFs used to sample the fluctuating velocities are Gaussian with a mean of zero and a variance of $\frac{2}{3}k$. As a result, there is a higher probability of particles traveling into the low kinetic energy region than there are traveling to the region of high kinetic energy, thus resulting in a net migration of particles to the region of low kinetic energy.

An analytical expression for the net flow of particles across the kinetic energy step function can be derived using the PDFs used to sample the fluctuating velocities. The first time step is only considered. Therefore, the concentration or number of particles (N) will be initially uniform. The net flow equation will take the form

$$\begin{aligned}\text{Net Flow} &= \text{Flow Up(from high } k \text{ region)} \\ &\quad - \text{Flow Down(from low } k \text{ region)} \\ &= \text{Probability(Flow Up)} * N \\ &\quad - \text{Probability(Flow Down)} * N. \end{aligned} \tag{8}$$

The probability of upward particle flow can be expressed as

$$\begin{aligned}&\text{Probability(Flow Up)} \\ &= P_{\text{high}}\left(v' > \frac{y_1}{\Delta t}\right) + P_{\text{high}}\left(v' > \frac{y_2}{\Delta t}\right) \\ &\quad + P_{\text{high}}\left(v' > \frac{y_3}{\Delta t}\right) + \cdots + P_{\text{high}}\left(v' > \frac{y_n}{\Delta t}\right) \\ &= \sum_{i=1}^{\infty} P_{\text{high}}\left(v' > \frac{y_i}{\Delta t}\right), \end{aligned} \tag{9}$$

where y_i is the distance of the ith control volume away from the kinetic energy step function. A similar expression can be derived for the downward flow of particles.

$$\text{Probability(Flow Down)} = \sum_{i=1}^{\infty} P_{\text{low}}\left(v' < \frac{-y_i}{\Delta t}\right). \tag{10}$$

The following is true because the PDF for v' is symmetric about zero:

$$\sum_{i=1}^{\infty} P_{\text{low}}\left(v' < \frac{-y_i}{\Delta t}\right) = \sum_{i=1}^{\infty} P_{\text{low}}\left(v' > \frac{y_i}{\Delta t}\right) \tag{11}$$

Using the above information, a revised expression for the net flow can be found:

$$\text{Net Flow} = N\left[\sum_{i=1}^{\infty}\left(P_{\text{high}}\left(v' > \frac{y_i}{\Delta t}\right) - P_{\text{low}}\left(v' > \frac{y_i}{\Delta t}\right)\right)\right]. \tag{12}$$

The probability functions can be substituted into the expression for the net flow

$$\text{Net Flow} = N\left[\sum_{i=1}^{\infty}\left(\int_{y_i/\Delta t}^{\infty} f_{\text{high}}(v')\,\mathrm{d}v' - \int_{y_i/\Delta t}^{\infty} f_{\text{low}}(v')\,\mathrm{d}v'\right)\right], \tag{13}$$

where $f_i(v') = \frac{2}{\sqrt{2\pi}\sigma}\mathrm{e}^{-\frac{1}{2}\left(\frac{v'}{\sigma_i}\right)^2}$ and $\sigma_i = \sqrt{\frac{2}{3}k_i}$ for the Shuen, Chen and Faeth [16] model.

Solving the integrals gives

$$\text{Net Flow} = \frac{N}{2}\left[\sum_{i=1}^{\infty}\left(\operatorname{erf}\left(\frac{y_i}{\sqrt{2}\Delta t\sigma_{\text{low}}}\right) - \left(\frac{y_i}{\sqrt{2}\Delta t\sigma_{\text{high}}}\right)\right)\right]. \tag{14}$$

The summation can be transformed into an integral by defining $N = \sum_{i=1}^{\infty} CA\Delta y_i$:

$$\text{Net Flow} = \frac{CA}{2}\left[\int_0^{\infty}\left(\operatorname{erf}\left(\frac{y_i}{\sqrt{2}\Delta t\sigma_{\text{low}}}\right) - \left(\frac{y_i}{\sqrt{2}\Delta t\sigma_{\text{high}}}\right)\right)\mathrm{d}y\right]. \tag{15}$$

Integrating and simplifying the above equation gives

$$\text{Net Flow} = \frac{CA}{\sqrt{2}}\left[\frac{\sigma_{\text{high}}\Delta t}{\sqrt{\pi}} - \frac{\sigma_{\text{low}}\Delta t}{\sqrt{\pi}}\right]. \tag{16}$$

This is the analytical prediction of the migration of particles after the first time step for the case of a uniform flow with two regions of uniform kinetic energy (step function). Eq. (16) indicates that as expected, the net flow increases with increasing inhomogeneity and increasing time step.

4.2. Case 2 – Gradual change in kinetic energy

The second test case has the same grid domain and particle injection scheme as the previous test case. The turbulence properties differ in terms of the kinetic energy profile such that a more gradual change in kinetic energy occurs:

$$k = \begin{cases} 0.1\ \mathrm{m^2/s^2} & \text{for } y < 2.5\ \mathrm{m}, \\ 0.45 + 0.35 * \sin\left(\left(\frac{\pi}{2}\right)(y - 3.5)\right)\ \mathrm{m^2/s^2} & \\ \quad \text{for } 2.5\ \mathrm{m} \leqslant y \leqslant 4.5\ \mathrm{m}, & \\ 0.8\ \mathrm{m^2/s^2} & \text{for } y > 4.5\ \mathrm{m}. \end{cases}$$

The kinetic energy profile is shown in Fig. 3. This case is designed to ensure a continuous kinetic energy gradient profile. Once again, the ratio of the kinetic energy to dissipation rate is kept constant to ensure a constant eddy lifetime and therefore a uniform time step.

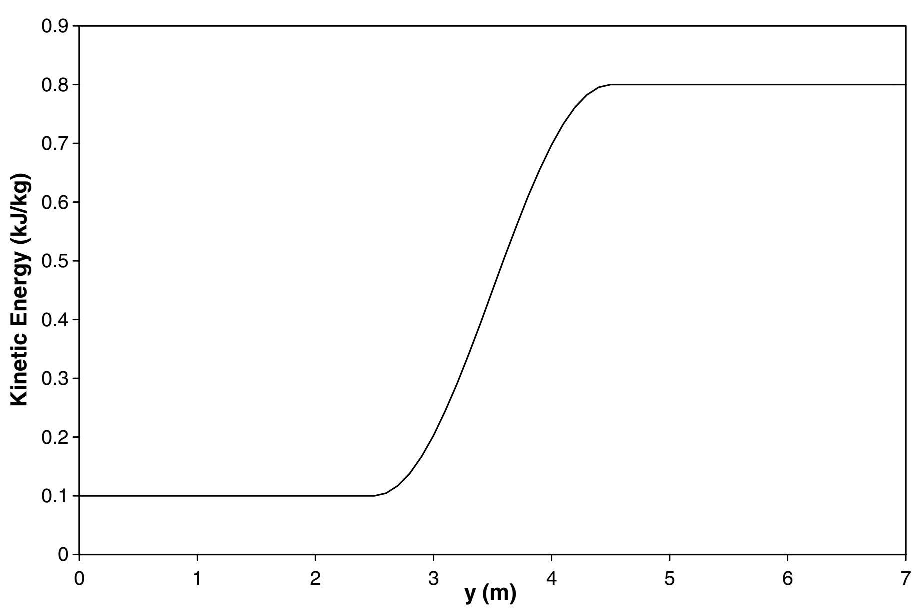

Fig. 3. Kinetic energy profile for the second test case.

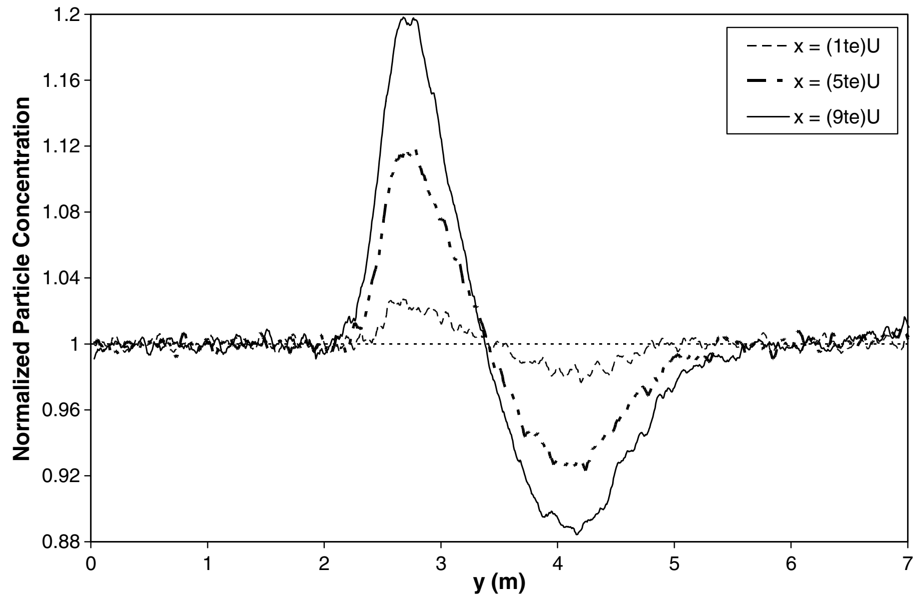

Fig. 4. Normalized particle concentration profiles for the second test case at different locations downstream from the inlet.

Fig. 4 is a plot of the normalized particle concentration profiles predicted by the Shuen, Chen and Faeth [16] model at several downstream locations. The model predicted a clear migration of particles from the region of high turbulent intensity to low turbulent intensity. In this case, the amplitude of the concentration profile reduced relative to case 1 since a continuous kinetic energy profile is applied as compared to the step function used in case 1. Once again, the particle migration is amplified downstream from the inlet.

5. Methods to correct for false particle migration

The false migration of fluid particles arises in the discontinuous random walk model because the turbulent fluctuation, determined at the start of the eddy lifetime, is held constant for the duration of the eddy lifetime. Researchers [1–3] have attempted to resolve this issue by adding a correction velocity and/or updating the turbulence intensity during the particle/eddy interaction.

5.1. MacInnes and Bracco

MacInnes and Bracco [1] combined updating the kinetic energy with a correction velocity. At each sub-time step, the following instantaneous fluctuating velocity is applied:

$$\vec{u}'_{\text{new}} = \vec{u}'_{\text{old}} \frac{\sqrt{\frac{2}{3}k_{\text{new}}}}{\sqrt{\frac{2}{3}k_{\text{old}}}} = \vec{\Gamma}\sqrt{\frac{2}{3}k_{\text{new}}}. \tag{17}$$

Note that the random variable Γ is held constant over the particle/eddy interaction time (as required by the discontinuous random walk model). The correction velocity was derived by estimating the mean fluctuating velocity from the characteristic distances particles travel during an eddy lifetime. Assuming a linearized variation in σ, isotropy and $\left|\frac{\mathrm{d}^2\sigma/\mathrm{d}x^2}{\mathrm{d}\sigma/\mathrm{d}x}\right|\sigma\tau_L < 1$, the transverse correction velocity can be written as

$$v'_c = \frac{1}{3}\frac{\partial k}{\partial y}t_e. \tag{18}$$

A similar correction can be applied to the streamwise and spanwise directions. The correction velocity is applied at the beginning of every particle/eddy interaction.

5.2. Chen

Chen [2] updated the turbulent intensity at time intervals that were much smaller than the eddy lifetime (or sub-time steps). Using an anisotropic discontinuous random walk model, Chen used the normal stress found from a second moment closure model to approximate the turbulence intensity. For this analysis isotropy will be assumed and the turbulence intensity will be approximated as $\sqrt{\frac{2}{3}k}$. As a result, this method reduces to updating the kinetic energy at every sub-time step.

5.3. Bocksell and Loth

Another correction velocity that is applied in conjunction with updating the kinetic energy is that of Bocksell and Loth [3]. Bocksell and Loth's correction velocity accounted for the particle acceleration due to the gradient in σ^2. This was done by analyzing the Lagrangian derivative of the fluid velocity along the fluid path. For isotropic, thin free-shear flows, the transverse correction velocity takes the form

$$v'_c(t+\Delta t) = v'_c(t) + \frac{1}{3}\frac{\partial k}{\partial y}\Delta t, \tag{19}$$

and is applied multiple times during a particle/eddy interaction. The above velocity corrections can also be applied in the streamwise and spanwise directions.

5.4. Strutt and Lightstone

Probability and statistics can also be used to derive a correction velocity. Consider an eddy of size l. For the case of inhomogeneous turbulence, there will be a gradient of the root mean square (rms) of the fluctuating velocity within the eddy. Using probability theory, an expected or mean value for the fluctuating velocity can be determined for both the upper and lower half of the eddy. For the Shuen, Chen and Faeth [16] model, the PDF for the fluctuating velocity is assumed to be Gaussian:

$$f(v') = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{v'}{\sigma}\right)^2}, \tag{20}$$

where the mean is zero and the standard deviation, σ, is $\sqrt{\frac{2}{3}k}$. The PDF for the negative fluctuating velocities only can be expressed as

$$f(v' : v' < 0) = \frac{2}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{v'}{\sigma}\right)^2}. \tag{21}$$

The mean or expected value of the negative fluctuating velocities can then be determined as

$$E(v') = \int_{-\infty}^{0} v' f(v' : v' < 0)\,\mathrm{d}v' = -\sigma\sqrt{\frac{2}{\pi}}, \tag{22}$$

and is the expected velocity of downward moving particles. Thus, the mean or expected value for the random fluctuating velocity for particles starting at the top of the eddy and moving down is

$$\overline{v'_{\text{top}}} = -\sqrt{\frac{2}{\pi}}\sigma|_{y+\frac{1}{2}l}. \tag{23}$$

After substituting in the standard deviation of the fluctuating velocity PDF, the expression for the average fluctuating velocity for the top half of the eddy becomes

$$\overline{v'_{\text{top}}} = -\sqrt{\frac{4}{3\pi}}\sqrt{k|_{y+\frac{1}{2}l}}. \tag{24}$$

A similar procedure can be used to derive an expression for the mean random fluctuating velocity for particles starting at the bottom of the eddy and moving up to give:

$$\overline{v'_{\text{bottom}}} = \sqrt{\frac{4}{3\pi}}\sqrt{k|_{y-\frac{1}{2}l}}. \tag{25}$$

The net flow of particles across the midsection of the eddy should be zero:

$$\overline{v'_{\text{top}}} + \overline{v'_{\text{bottom}}} = 0. \tag{26}$$

Therefore, a correction to the velocities needs to be added such that the mean net flow at y will be zero:

$$\overline{v'_{\text{top}}} + \overline{v'_{\text{bottom}}} + v'_c = 0, \tag{27}$$

$$v'_c = -(\overline{v'_{\text{top}}} + \overline{v'_{\text{bottom}}}). \tag{28}$$

Substituting in the expression for the fluctuating velocity at the top and bottom of the eddy, the correction velocity takes the form

$$v'_c = \sqrt{\frac{4}{3\pi}}\left(\sqrt{k|_{y+\frac{1}{2}l}} - \sqrt{k|_{y-\frac{1}{2}l}}\right). \tag{29}$$

If it is assumed that over the length of an eddy $\sqrt{k}$ varies linearly with position, the correction velocity becomes

$$v'_c = \sqrt{\frac{1}{3\pi}}\frac{1}{\sqrt{k}}\frac{\mathrm{d}k}{\mathrm{d}y}l. \tag{30}$$

In order to apply this correction factor to the test cases, the value of l that corresponds to a given time step needs to be found. By using the expected value for the fluctuating velocities, the length scale can be approximated by

$$l = v'_{avg}\Delta t = \sqrt{\frac{2}{\pi}}\sigma\Delta t. \tag{31}$$

Using this form of the length scale gives

$$v'_c = 0.212\frac{\mathrm{d}k}{\mathrm{d}y}\Delta t. \tag{32}$$

The accuracy of this correction velocity should increase as the length or time step decreases. Strutt and Lightstone [17] found the general form of the correction can be written as

$$v'_{c_i} = 0.212\left.\frac{\mathrm{d}k}{\mathrm{d}y}\right|_{y_i}\Delta t_{\text{sub}} + v'_{c_{i-1}}. \tag{33}$$

This correction velocity will be implemented in much the same way as the correction velocity proposed by Bocksell and Loth [3]. Due to the inherent assumption of isotropy in the Shuen, Chen and Faeth [16] model, the correction velocity for all three directions takes the same form.

6. Analysis of the different correction methods

There are two different correction methods that are typically applied to the discontinuous random walk model: updating the kinetic energy and/or adding a correction velocity to the mean velocity. The updating the kinetic energy method is analyzed and is found to have limited effectiveness. The performance of the correction velocities are then compared using the second test case that involves a gradual change in the kinetic energy.

6.1. Updating kinetic energy method adapted from Chen [2]

An intuitive solution is to apply the local value of the turbulent kinetic energy at sub-time steps of the eddy lifetime. As the sub-time step is reduced, it is expected that the false migration will no longer occur. This proposed correction for the false particle migration is tested for the second idealized inhomogeneous turbulence test case. Fig. 5 compares the normalized particle concentration profile obtained with no correction and with updating the kinetic

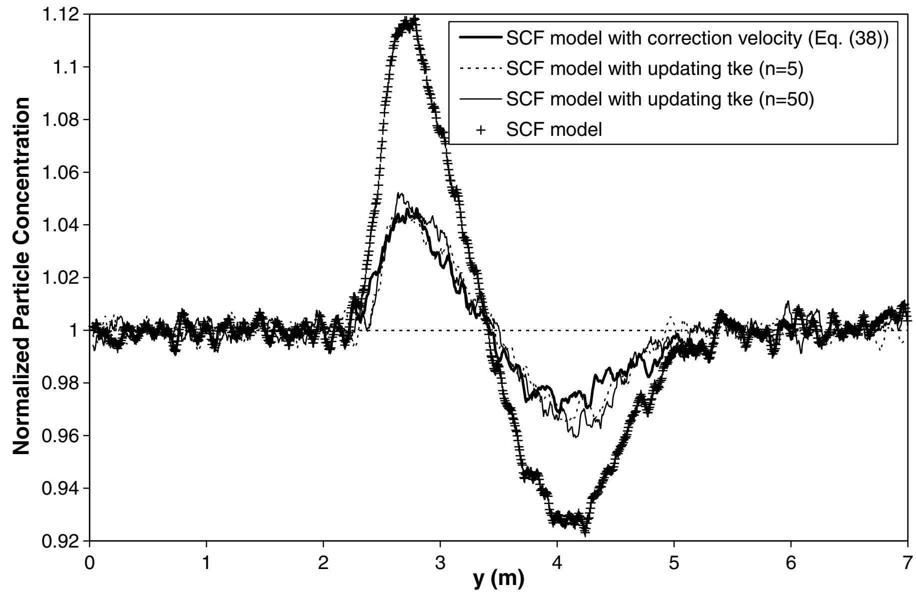

Fig. 5. Normalized particle concentration profiles predicted from the Shuen, Chen and Faeth [16] model for the second test case at $x = (5t_e)U$.

energy using multiple numbers of sub-steps for the second test case. The results show that although the particle migration is reduced, the updating kinetic energy method appears to reach an effective limit quickly as the time step is reduced and also fails to remove the false migration of particles.

Updating the kinetic energy at every sub-time step can be shown to be equivalent to applying a correction velocity to the initial turbulent fluctuation. By putting the updating kinetic energy method in this context, it helps explain the limited effectiveness of this method as well as allows for a direct comparison with other proposed correction velocities.

6.1.1. Effective correction velocity over sub-time step

The updating kinetic energy method takes the form

$$v'_{\text{new}} = v'_{\text{old}}\left(\frac{\sigma_{\text{new}}}{\sigma_{\text{old}}}\right). \tag{34}$$

The 'new' standard deviation can be approximated by a first order Taylor series as

$$\sigma_{\text{new}} = \sigma_{\text{old}} + \left(\frac{d\sigma}{dy}\right)\bigg|_{\text{old}} \Delta y \tag{35}$$

or

$$\sigma_{\text{new}} = \sigma_{\text{old}} + \left(\frac{d\sigma}{dy}\right)\bigg|_{\text{old}} v'_{\text{old}}\Delta t. \tag{36}$$

Substituting in the expression for the standard deviation, $\sigma_i = \sqrt{\frac{2}{3}k_i}$, gives

$$v'_{\text{new}} = v'_{\text{old}} + \frac{1}{2}\left(\frac{1}{k}\right)\left(\frac{dk}{dy}\right)\left(v'_{\text{old}}\right)^2\Delta t. \tag{37}$$

The second term on the right hand side is essentially the correction velocity due to the updating kinetic energy method. Taking the average of the correction velocity (noting that $\overline{\left(v'_{\text{old}}\right)^2} = \frac{2}{3}k$) gives:

$$\overline{v'_{c,\text{sub}}} = \frac{1}{3}\left(\frac{dk}{dy}\right)\Delta t, \tag{38}$$

where $\overline{v'_{c,\text{sub}}}$ is the effective correction velocity equivalent to updating the kinetic energy at every sub-time step. Note that this correction velocity is applied at each sub-time step.

To test the validity of Eq. (38), simulations were performed using this correction velocity for test case two. Fig. 5 compares the results from the Shuen, Chen and Faeth model with the effective correction velocity (Eq. (38)) and with updating the kinetic energy. The two curves are very similar. This provides confidence in the analysis that indicates that the updating kinetic energy method is equivalent to adding a correction velocity.

The Bocksell and Loth [3] correction velocity is identical to that of the effective correction velocity (Eq. (38)) which was shown herein to be equivalent to updating the kinetic energy at every sub-time step. However, because the correction velocity of Bocksell and Loth is applied in conjunction with updating the kinetic energy, their correction is effectively twice that obtained by simply updating the kinetic energy.

6.1.2. Effective correction velocity over eddy lifetime

It is of interest to derive an average velocity correction applied over the eddy lifetime. This is done by firstly considering a case with a finite number of time steps (five in this example). The example is then extended to an arbitrary number (N). Initially the fluctuating velocity is v'. Therefore the first time step will use a fluctuating velocity of

$$v'_1 = v'. \tag{39}$$

For the second sub-time step, the fluctuating velocity will take the form

$$v_2' = v_1' + v_{c1}' \tag{40}$$

where v_{c1}' is the velocity correction equivalent to updating the kinetic energy. The third, fourth and fifth sub-time steps follow suit.

The distance a particle travels over an eddy lifetime can be written as follows:

$$\Delta y_{\text{tot}} = \sum_{i=1}^{5} \Delta y_i = \sum_{i=1}^{5} v_i' \Delta t, \tag{41}$$

where

$$\Delta t = \frac{t_{\text{e}}}{n+1}, \tag{42}$$

and n is the number of corrected sub-steps (in this case $n = 4$). Recall that the first sub-step is not corrected. Substituting the fluctuating velocities into Eq. (41) and simplifying gives

$$\Delta y_{\text{tot}} = 5v'\Delta t + (4v_{c1}' + 3v_{c2}' + 2v_{c3}' + v_{c4}')\Delta t. \tag{43}$$

The first term on the right hand side is the distance a particle travels without a correction during the eddy lifetime, $\Delta y|_{\text{nocorr}} = v' t_{\text{e}}$. The second term on the right-hand side must then be the distance traveled by a particle due to the correction over an eddy lifetime and it can be transformed into a series, where the number of sub-time steps $(n+1)$ is now generalized:

$$\Delta y|_{\text{corr}} = \sum_{i=1}^{n} (n+1-i) v_{ci}' \Delta t. \tag{44}$$

The distance traveled during a full time step due to the updating kinetic energy method can be expressed in terms of an average correction velocity as follows:

$$\Delta y|_{\text{corr}} = \overline{v_c'} t_{\text{e}}. \tag{45}$$

Combining the two expressions for $\Delta y|_{\text{corr}}$ gives

$$\overline{v_c'} = \frac{\sum_{i=1}^{n} (n+1-i) v_{ci}' \Delta t}{t_{\text{e}}}. \tag{46}$$

After substituting the effective correction velocity over the sub-time step (Eq. (38)) into the above equation and assuming constant $\frac{\mathrm{d}k}{\mathrm{d}y}$ the relationship becomes

$$\overline{v_c'} = \frac{1}{3t_{\text{e}}} \left(\frac{\mathrm{d}k}{\mathrm{d}y}\right) \left[\sum_{i=1}^{n} (n+1)\Delta t^2 - \sum_{i=1}^{n} i \Delta t^2\right]. \tag{47}$$

Using Eq. (42) and

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2}, \tag{48}$$

the average correction velocity takes the form

$$\overline{v_c'} = \frac{1}{6} \frac{\mathrm{d}k}{\mathrm{d}y} \{t_{\text{e}} - \Delta t\}. \tag{49}$$

As $\Delta t \to 0$, the average corrected velocity (over the eddy lifetime) is

$$\overline{v_c'} = \frac{1}{6} \frac{\mathrm{d}k}{\mathrm{d}y} t_{\text{e}}. \tag{50}$$

The limit given by Eq. (49) can be reached relatively quickly. For example, for a constant kinetic energy gradient case, the difference in the average correction between 50 sub-steps and 100 sub-steps is 1%.

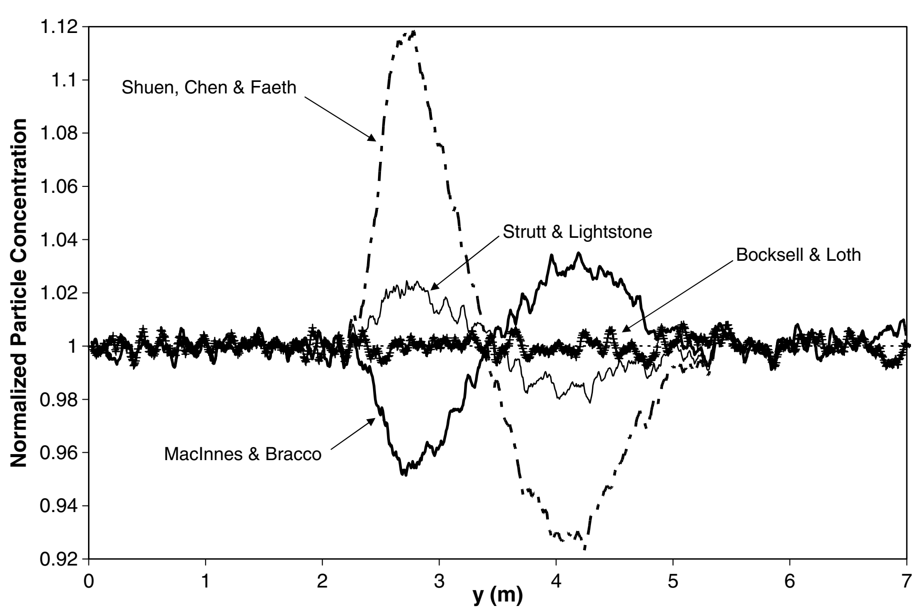

Fig. 6. Comparison of correction factors for the second test case at $x = (5t_{\text{e}})U$.

The results show that updating the kinetic energy has a limited effectiveness. This indicates the need for an additional correction. This would explain why researchers such as MacInnes and Bracco [1] and Bocksell and Loth [3] have proposed corrections that involved both updating the kinetic energy and applying a correction velocity.

6.2. 'Correction' velocities

Fig. 6 compares the normalized particle concentration curves that were obtained when the MacInnes and Bracco [1], Bocksell and Loth [3] and the Strutt and Lightstone [17] correction factors were applied to the second test case after 5 eddy lifetimes. All three correction factors take similar forms, however, they differ in the empirical constant used and the frequency at which they are applied. The MacInnes and Bracco correction over corrects for the particle migration while the Strutt and Lightstone correction under corrects. The Bocksell and Loth correction performs the best out of all the corrections producing a fairly uniform normalized particle concentration curve of approximately one.

7. Conclusion

SSF models predict unphysical results for tracer particles in inhomogeneous turbulence due to the way in which the fluctuating velocities are modeled. Because the PDF's, used to sample the fluctuating velocity, have a standard deviation that is related to the kinetic energy, there is a higher probability of particles traveling to regions of low turbulence intensity than traveling to regions of high turbulence intensity. The problem is amplified by the fact that the fluctuating velocity is held constant for the duration of the particle/eddy interaction.

A correction that involves updating the kinetic energy (and thus the fluctuating component of the velocity) multiple times during an eddy lifetime was tested. It was hypothesized that as the number of sub-steps increases, the particle migration would reduce and there would be no need for a corrective velocity. Indeed, previous researchers have used this approach to account for inhomogeneity.

The updating kinetic energy method consistently failed to completely correct for the particle migration. In order to explain the apparent limit of the updating kinetic energy methods corrective ability, an estimate for the average correction over an eddy lifetime that is equivalent to the updating kinetic energy method was found. This average correction converges quickly as the timestep is reduced, and it was found that further correction was required. For the test cases considered herein, the correction of Bocksell and Loth [3] was the most effective in reducing the false migration of particles.

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