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Second-order modelling of particle dispersion in a turbulent flow

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A set of second-order modelled equations for the motion of particles are presented. We consider the effects of the particle inertia and the crossing-trajectories effect on the particle dispersion. A simple case of a particle mixing layer in a decaying homogeneous turbulence for light and heavy particles is calculated. The results show that the crossing-trajectories effect on particle dispersion is very significant, while inertia only has a slight effect. This behaviour has been observed in experiments (Wells & Stock 1983) and is well predicted by an asymptotic analysis (Csanady, 1963). The calculation also shows that there is a significant difference between Favre-averaged particle velocity and conventional-averaged particle velocity in the low-particle-concentration region. All calculations are in good agreement with Wells & Stock's experimental data.

1. Introduction

The study of particle behaviour in a turbulent flow is often of importance: it may help us to predict the dispersal of contaminants in the atmosphere and ocean, and may also be important in LDA measurements in which the effect of concentration fluctuations of the seeding particles on the measurement of turbulence statistics may be significant.

Although the concentration of particles in a fluid is a scalar, its behaviour is quite different from other scalars (temperature, moisture, gas species etc.) because of inertia and the crossing-trajectories effect (Yudine 1959). The behaviour of scalars such as temperature and moisture in a turbulent flow has been extensively studied with both experiments and theoretical models; the behaviour of particles has been studied less (Csanady 1963; Snyder & Lumley 1971; Meek & Jones 1973; Lumley 1978*c*; Nir & Pismen 1979; Wells & Stock 1983; Lottey, Lumley & Shih 1983).

The influence of the crossing-trajectories effect is quite clear: it decreases the particle dispersion, because the particles fall from one eddy to another, so that the correlations between particle and fluid velocities decreases. However, the effect of the particle inertia is not so clear. The inertia effect is mainly represented by the particle time constant. Csanady (1963) showed that an asymptotic (i.e. long-time) particle diffusivity is independent of the particle time constant. Wells & Stock's (1983) experiments also show that there is not a large difference of diffusivity between light particles and heavy particles, although there is an indication that the diffusivity of the heavy particles is a little larger than that of the light particles. Our second-order modelling calculations predict this observed behaviour.

In this paper we first derive a set of second-order modelled equations under the conditions that the concentration of particles is small enough (say, less than 0.003, Lumley 1978*c*) so that the particles can be considered as non-interactive, and that the timescale ratio (the ratio of the particle time constant to the Kolmogorov timescale) and the lengthscale ratio (the ratio of the particle size to the Kolmogorov lengthscale) are small. The influence of inertia and the crossing-trajectories effect on the particle diffusion are considered. Secondly, we describe the models required by the closure. Finally we carry out calculations of a particle mixing layer for the light and heavy particles used by Snyder & Lumley (1971) and Wells & Stock (1983) in their experiments. The calculations show that the crossing-trajectories effect indeed dominates the particle dispersion. The influence of the particle inertia appears to increase only slightly the effective diffusivity even for heavy particles. All the calculations compare favourably with the experimental data of Wells & Stock (1983).

In addition to the particle dispersion, we also calculate the difference between Favre-averaging and conventional averaging for the particle velocity and the variance of the particle-velocity fluctuations. The particle-velocity differences between Favre-averaging and conventional averaging are significant, especially in the low-concentration region, but there are no significant velocity-variance differences between the two averaging methods. These results are relevant for the analysis of LDA measurements.

2. Basic equation

Let us consider a fluid with local velocity u_i and constant density ρ, containing a monodisperse cloud of undeformable particles having radius σ. The volume fraction is considered to be so small (say, less than 0.003) that the interaction between individual particles may be neglected (Lumley 1978*c*). The particles are assumed to be too large for Brownian motion to be important. We must also assume the particles are small enough compared to the Kolmogorov microscale so that the flow about a particle is nearly a simple shear. We consider the particle cloud as a continuum (Lumley 1978*c*), at least on scales of the energy-containing range. In geophysical situations, the above assumptions are true for naturally occurring aerosols and fogs in turbulent flow. For some other situations, say foams and slurries, there exist strong interactions between particles. Here we only deal with situations in which the particle cloud can be considered as a non-interacting continuum. Hence, the particles only interact with the fluid. In general the equation of motion of a particle is extremely complicated. However, if the relative Reynolds number (based on terminal velocity and particle size) is less than $\frac{1}{2}$, the size of particles σ is small relative to the Kolmogorov lengthscale η and the particle time constant τ_p is short relative to the Kolmogorov timescale τ_k, then the equation of motion of a particle can be rigorously written as (Lumley 1978*c*)

$$\dot{u}_{pi} + u_{pi,j}\, u_{pj} = (u_i - u_{pi})/\tau_p + g_i, \tag{1}$$

where u_{pi} represents the particle velocity, u_i is the fluid velocity, g_i is the gravity vector and τ_p is the particle time constant, given by (according to Stokes flow)

$$\tau_p = m_p/6\pi\sigma\mu.$$

Here and throughout we have taken the density of particle material to be large relative to fluid density, for simplicity. Factors depending on the density ratio may easily be introduced, modifying g_i and τ_p to restore the general case. Here m_p is the mass of a particle, σ is the radius of the particle and μ is the viscosity. If we define

	Hollow glass	Solid glass	Corn	Copper
Diameter (μm)	46.5	87.0	87.0	46.5
Density (g/cm³)	0.26	2.5	1.0	8.9
Time constant (ms)†	1.7	45.0	20.0	49.0
Timescale ratio‡	0.145	3.85	1.72	4.21
Lengthscale ratio‖	0.105	0.198	0.198	0.105
Stokes velocity (cm/s)	1.67	56.2	22.5	57.0
Terminal velocity (cm/s)¶	1.67	44.2	19.8	48.3
Reynolds number	0.05	2.48	1.10	1.45

† Based on terminal velocity; ‡ the fluid timescale is 11.6 ms at $x/M = 73$; ‖ the Kolomogorov microscale is 0.043 cm at $x/M = 73$; ¶ computed from table 5 in Fuchs (1964, p. 32).

TABLE 1. Particles and relevant parameters

Parameter	5 μm glass sphere	57 μm glass sphere
Diameter (μm)	5	57
Density (kg/m)	2475	2420
τ_p (ms)	0.192	24.4
τ_p/τ_k†	2.34×10^{-2}	2.972
q_p (coulomb)	1.66×10^{-15}	9.71×10^{-14}
Stokes velocity (cm/s)	0.188	23.26
Terminal velocity (cm/s)	0.188	23.16
Reynolds number	6.30×10^{-3}	0.887

† $\tau_k = 8.21 \times 10^{-3}$ s at $x/M = 45$.

TABLE 2. Particle data

c as the mass of particles per unit volume, or simply call it particle density, then we may write a conservation equation as

$$\dot{c} + (cu_{pi})_{,i} = 0. \tag{2}$$

For the equation of fluid motion, we should consider the force exerted upon a unit volume of fluid by the particles. The force exerted on the fluid by a unit mass of particles is $(u_{pi} - u_i)/\tau_p$, so that the volumetric force exerted by the particles is $c(u_{pi} - u_i)/\tau_p$ and the equation of fluid motion can be written as

$$\dot{u}_i + u_j u_{i,j} = -\frac{1}{\rho} p_{,i} + \frac{c}{\rho} \frac{u_{pi} - u_i}{\tau_p} + \nu u_{i,jj}. \tag{3}$$

Conservation of mass for the fluid is

$$u_{i,i} = 0. \tag{4}$$

Equations (1)–(4) are the basic equations for the instantaneous quantities c, u_{pi}, u_i and p. The restrictions on (1) are Stokes flow around the particle and small timescale ratio of τ_p/τ_k. Tables 1 and 2 are the particle data taken from Snyder & Lumley (1971) and Wells & Stock (1983). From these tables we can see that (1) is only valid for light particles (hollow glass and 5 μm glass sphere). For heavy particles (say, 87 μm glass and 57 μm glass for which the timescale ratio > 3) (1) is doubtful. However, the range of validity of (1) can be extended to a relative Reynolds number of 10 (which corresponds to a heavy particle) by using different time constants in the vertical and horizontal directions (Lumley 1978*c*).

If the inertia term (left-hand side of (1)) can be neglected under some circumstances (Lumley 1978*c*) then we obtain the solution for the particle velocity u_{pi}

$$u_{pi} = u_i + \tau_p g_i. \tag{5}$$

The equation of fluid motion becomes

$$\dot{u}_i + u_{i,j} u_j = -\frac{1}{\rho} p_{,i} + \frac{c}{\rho} g_i + \nu u_{i,jj}, \tag{6}$$

and (2) becomes

$$\dot{c} + (u_i + \tau_p g_i) c_{,i} = 0. \tag{7}$$

Equations (5)–(7) are suitable for the case of atmospheric aerosol particles (Lottey *et al.* 1983). Now if we want to include the effect of inertia, then (5) must be modified. We know that τ_p is smaller than the Kolmogorov timescale τ_k, which is the smallest timescale in the turbulence. We may expand u_{pi} in terms of τ_p as follows:

$$u_{pi} = u_i + u_i^{(1)} \tau_p + \dots. \tag{8}$$

Substituting (8) into (1) gives, for $u_i^{(1)}$,

$$u_i^{(1)} = -(\dot{u}_i + u_j u_{i,j}) + g_i,$$

and the solution of u_{pi} is, instead of (5),

$$u_{pi} = u_i - \tau_p(\dot{u}_i + u_j u_{i,j}) + \tau_p g_i + O(\tau_p^2). \tag{9}$$

Substituting (9) into (3), we obtain

$$\left(1 + \frac{c}{\rho}\right)(\dot{u}_i + u_{i,j} u_j) = -\frac{1}{\rho} p_{,i} + \frac{c}{\rho} g_i + \nu u_{i,jj}, \tag{10}$$

and (2) will become (using (9) in (2))

$$\dot{c} + (u_i + \tau_p g_i) c_{,i} = \tau_p [c(u_i + u_j u_{i,j})]_{,i}. \tag{11}$$

At this point we should note that (9) is useful for forming correlations between particle and other quantities, but not for the particle Reynolds stress and particle turbulent energy, because (1) under the approximation (9) implies $\mathrm{D}u_{pi}/\mathrm{D}t = \mathrm{D}u_i/\mathrm{D}t$, and this means no difference between particles and fluid for Reynolds stress and turbulent energy.

If the density ratio c/ρ is small then the fluid motion will be approximately unchanged by the presence of the particles, i.e.

$$\dot{u}_i + u_{i,j} u_j = -\frac{1}{\rho} p_{,i} + \nu u_{i,jj}. \tag{12}$$

We will use (9), (11) and (12) to study particle dispersion with the restriction to Stokes particles in mind.

By using the following Reynolds decomposition

$$u_{pi} = \overline{U}_{pi} + u'_{pi}, \quad u_i = \overline{U}_i + u'_i, \quad p = \overline{p} + p', \quad c = \overline{c} + c'$$

from (12) we obtain

$$\dot{\overline{U}}_i+\overline{U}_j\overline{U}_{i,j}+(\overline{u_i'u_j'})_{,j}=-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}, \tag{13}$$

$$\dot{u}_i'+\overline{U}_j u_{i,j}'+u_j'\overline{U}_{i,j}+u_j'u_{i,j}'-(\overline{u_i'u_j'})_{,j}=-\frac{1}{\rho}p_{,i}'+\nu u_{i,jj}', \tag{14}$$

and, from (9),

$$\overline{U}_{pi}=\overline{U}_i+\frac{\tau_p}{\rho}\overline{p}_{,i}+V_{pi}, \tag{15}$$

$$u_{pi}'=u_i'-\tau_p\left[-\frac{1}{\rho}p_{,i}+\nu u_{i,jj}\right], \tag{16}$$

where $V_{pi}\equiv\tau_p g_i$, which is called the particle terminal velocity.

From (11),

$$\dot{\overline{C}}+(\overline{U}_i+V_{pi})\overline{C}_{,i}+(\overline{cu_i})_{,i}=\tau_p\left[-\frac{\overline{C}}{\rho}\overline{p}_{,i}-\frac{1}{\rho}\overline{c'p'_{,i}}+\nu\overline{c'u'_{i,jj}}\right]_{,i}, \tag{17}$$

$$\begin{aligned}\dot{c}'+\overline{U}_i c'_{,i}+u_i'\overline{C}_{,i}+u_i'c'_{,i}-\overline{u_i'c'_{,i}}+V_{pi}c'_{,i}\\ =\tau_p\Big[\overline{C}_{,i}\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)+\overline{C}\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)_{,i}+c'_{,i}\Big(-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}\Big)\\ +c'\Big(-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}\Big)_{,i}+c'_{,i}\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)\\ +c'\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)_{,i}+\Big(\frac{1}{\rho}\overline{c'p'_{,i}}-\nu\overline{c'u'_{i,jj}}\Big)_{,i}\Big].\end{aligned}$$

Note:

$$\Big(-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}\Big)_{,i}=\overline{U}_{j,i}\overline{U}_{i,j}+(u_i'u_j')_{,ij};$$

$$\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)_{,i}=\overline{U}_{j,i}u'_{i,j}+u'_{j,i}\overline{U}_{i,j}+u'_{j,i}u'_{i,j}-(\overline{u_i'u_j'})_{,ij},$$

so that

$$\begin{aligned}\dot{c}'+(\overline{U}_i+V_{pi})c'_{,i}+u_i'\overline{C}_{,i}+u_i'c'_{,i}\\ =\tau_p\Big[\overline{C}_{,i}\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)+\overline{C}(\overline{U}_{j,i}u'_{i,j}+u'_{j,i}\overline{U}_{i,j}+u'_{j,i}u'_{i,j})\\ +c'_{,i}\Big(-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}\Big)+c'(\overline{U}_{j,i}\overline{U}_{i,j}+(\overline{u_i'u_j'})_{,ij})\\ +c'_{,i}\Big(-\frac{1}{\rho}p'_{,i}+\nu u'_{i,jj}\Big)+c'(\overline{U}_{j,i}u'_{i,j}+u'_{j,i}\overline{U}_{i,j}+u'_{j,i}u'_{i,j}-(\overline{u_i'u_j'})_{,ij}\Big].\end{aligned} \tag{18}$$

We may form from (18)

$$\begin{aligned}\dot{\overline{c'^2}}+(\overline{U}_i+V_{pi})\overline{c'^2}_{,i}+2\overline{c'u_i'}\overline{C}_{,i}+(\overline{c'^2u_i'})_{,i}\\ =2\tau_p\Big[\overline{C}_{,i}\Big(-\frac{1}{\rho}\overline{p'_{,i}c'}+\nu\overline{c'u'_{i,jj}}\Big)\\ +\overline{C}(2\overline{U}_{j,i}\overline{c'u'_{i,j}}+\overline{c'u'_{j,i}u'_{i,j}})+\frac{\overline{c'^2}_{,i}}{2}\Big(-\frac{1}{\rho}\overline{p}_{,i}+\nu\overline{U}_{i,jj}\Big)+\overline{c'^2}\,\overline{U}_{j,i}\overline{U}_{i,j}\\ +\frac{1}{2}\Big(-\frac{1}{\rho}\overline{p'_{,i}c'^2_{,i}}+\nu\overline{c'^2_{,i}u'_{i,jj}}\Big)+2\overline{U}_{j,i}\overline{c'^2u'_{i,j}}+\overline{c'^2u'_{j,i}u'_{i,j}}\Big].\end{aligned}$$

Note: $$\frac{1}{2}\left(-\frac{1}{\rho}\overline{p'_{,i}c'^2_{,i}}+\nu\overline{c'^2_{,i}u'_{i,jj}}\right)=\frac{1}{2}\left(-\frac{1}{\rho}\overline{p'_{,i}c'^2}+\nu\overline{c'^2u'_{i,jj}}\right)_{,i}+\frac{1}{2\rho}\overline{c'^2p'_{,ii}},$$

and, from (14),

$$\frac{1}{2\rho}\overline{c'^2p'_{,ii}}=-\tfrac{1}{2}(\overline{U}_{j,i}\overline{c'^2u'_{i,j}}+\overline{U}_{i,j}\overline{c'^2u'_{j,i}}+\overline{c'^2(u'_iu'_j)_{,ij}}-\overline{c'^2(u'_iu'_j)_{,ij}})$$
$$=-\overline{U}_{j,i}\overline{c'^2u'_{i,j}}+\tfrac{1}{2}\overline{c'^2(u'_iu'_j)_{,ij}}-\tfrac{1}{2}\overline{c'^2u'_{i,j}u'_{j,i}}.$$

Finally we obtain

$$\dot{\overline{c'^2}}+(\overline{U}_i+V_{pi})\overline{c'^2}_{,i}+2\overline{c'u'_i}\,\overline{C}_{,i}+(\overline{c'^2u'_i})_{,i}$$
$$=2\tau_p\Big[\overline{C}_{,i}\Big(-\frac{1}{\rho}\overline{p'_{,i}c'}+\nu\overline{c'u'_{i,jj}}\Big)+\overline{C}(2\overline{U}_{j,i}\overline{c'u'_{i,j}}+\overline{c'u'_{j,i}u'_{i,j}})$$
$$+\tfrac{1}{2}\bar{c}^2_{,i}\Big(-\frac{1}{\rho}\overline{P}_{,i}+\nu\overline{U}_{i,jj}\Big)+\bar{c}^2\overline{U}_{j,i}\overline{U}_{i,j}+\frac{1}{2}\Big(-\frac{1}{\rho}\overline{p'_{,i}c'^2}+\nu\overline{c'^2u'_{i,jj}}\Big)_{,i}$$
$$+\overline{U}_{j,i}\overline{c'^2u'_{i,j}}+\tfrac{1}{2}(\overline{c'^2(u'_iu'_j)_{,ij}}+\overline{c'^2u'_{j,i}u'_{i,j}})\Big]-2\bar{\epsilon}_c,$$

where $\bar{\epsilon}_c$ is the dissipation rate of $\overline{c'^2}$. For the flux, we may form

$$\dot{\overline{c'u_i}}+\overline{u'_iu'_j}\,\overline{C}_{,j}+\overline{c'u'_j}\,\overline{U}_{i,j}+\overline{U}_j(\overline{c'u'_i})_{,j}+(\overline{c'u'_iu'_j})_{,j}+\overline{c'_{,j}u_i}\,V_{pj}$$
$$=-\frac{1}{\rho}\overline{p'_{,i}c'}+\nu\overline{c'u'_{i,jj}}+\tau_p\Big[\overline{C}_{,k}\Big(-\frac{1}{\rho}\overline{p'_{,k}u'_i}+\nu\overline{u'_iu'_{k,jj}}\Big)$$
$$+\overline{C}(\overline{U}_{j,k}\overline{u'_iu'_{k,j}}+\overline{u'_iu'_{j,k}}\,\overline{U}_{k,j}+\overline{u'_iu'_{j,k}u'_{k,j}})+\overline{u'_ic'_{,k}}\Big(-\frac{1}{\rho}\overline{P}_{,k}+\nu\overline{U}_{k,jj}\Big)$$
$$+\overline{c'u'_i}(\overline{U}_{j,k}\overline{U}_{k,j})+\Big(-\frac{1}{\rho}\overline{p'_{,k}c'_{,k}u'_i}+\nu\overline{u'_ic'_{,k}u'_{k,jj}}\Big)$$
$$+(2\overline{U}_{j,k}\overline{c'u'_iu'_{k,j}}+\overline{c'u'_iu'_{j,k}u'_{k,j}})\Big].$$

If we assume local isotropy for third- or higher-order moments at high turbulent Reynolds number $Re \gg 1$, then we obtain

$$\dot{\overline{c'u'_i}}+\overline{U}_j(\overline{c'u'_i})_{,j}+\overline{u'_iu'_j}\,\overline{C}_{,j}+\overline{c'u'_j}\,\overline{U}_{i,j}+(\overline{c'u'_iu'_j})_{,j}+\overline{c'_{,j}u'_j}\,V_{pj}$$
$$=-\frac{1}{\rho}\overline{p'_{,i}c'}+\nu\overline{c'u'_{i,jj}}+\tau_p\Big\{\overline{C}_{,k}\Big[-\frac{1}{\rho}\overline{p'_{,k}u'_i}-\nu\overline{u'_{i,j}u'_{k,j}}\Big]$$
$$-\frac{\overline{u'_ic'_{,k}}\,\overline{P}_{,k}}{\rho}+\overline{c'u'_i}\,\overline{U}_{j,k}\overline{U}_{k,j}+2\overline{U}_{j,k}\overline{c'u'_iu'_{k,j}}\Big\}. \tag{20}$$

The Reynolds-stress equations are unchanged:

$$\dot{\overline{u'_iu'_j}}+\overline{U}_k(\overline{u'_iu'_j})_{,k}+\overline{u_iu_k}\,\overline{U}_{j,k}+\overline{u_ju_k}\,\overline{U}_{i,k}+(\overline{u'_iu'_ju'_k})_{,k}$$
$$=-\frac{1}{\rho}(\overline{p'_{,i}u'_j}+\overline{p'_{,j}u'_i})+\nu(\overline{u'_iu'_{j,kk}}+\overline{u'_ju'_{i,kk}}). \tag{21}$$

In (19) we have introduced a dissipation term $\bar{\epsilon}_c$. Its exact mechanism is not clear, but, in order to reflect the fact that the particle-density fluctuations must be suppressed on a scale smaller than the interparticle distance (i.e. to avoid an ultraviolet catastrophe), such a term is required (Lottey *et al.* 1983). Such a term is also necessary to prevent unbounded growth of particle-concentration-fluctuation variance, another aspect of the same phenomenon. Therefore we need equations for $\bar{\epsilon}_c$ and $\bar{\epsilon}$, scalar dissipation and mechanical dissipation rate respectively. They can be written as:

$$\dot{\bar{\epsilon}}_c + (\bar{U}_j + \bar{V}_{pj})\,\bar{\epsilon}_{c,j} + (\overline{\epsilon_c' u_j'})_{,j} = -\frac{\bar{\epsilon}_c^2}{\overline{c'^2}}\psi^c; \tag{22}$$

$$\dot{\bar{\epsilon}} + \bar{U}_j\,\bar{\epsilon}_{,j} + (\overline{\epsilon' u_j'})_{,j} = -\frac{\bar{\epsilon}^2}{\overline{q^2}}\,\psi. \tag{23}$$

All the (unknown) physics in these general transport equations is hidden in the dimensionless terms ψ and ψ^c, which must be modelled on a more-or-less empirical basis. The equations (17), (19), (20), (21) and (23) are the bases on which we study the behaviour of particles in a turbulent flow. This set of equations does not include the effects of the presence of particles on the fluid turbulence. In principle there is no great difficulty in including these effects by starting again from (10). We believe that the equations we have derived above are suitable for studying the most important aspect of particle behaviour – dispersion.

3. Models

Now let us consider a decaying homogeneous isotropic turbulence in which there are no mean-velocity or mean-pressure gradients. In this case, the terms which must be modelled are the following:

3.1. *Pressure correlation terms*

In the present flow, we may model them as (Shih & Lumley 1981)

$$-\frac{1}{\rho}\overline{c'p'_{,i}} + \nu\,\overline{c'u'_{i,jj}} = \tfrac{1}{5}(\overline{q^2c'})_{,i} - \phi^c\,\overline{cu_i}\,\frac{\bar{\epsilon}}{\overline{q^2}},$$

$$-\frac{1}{\rho}\overline{p'_{,k}u'_i} - \nu\,\overline{u'_{i,j}u'_{k,j}} = -\tfrac{1}{3}\bar{\epsilon}\delta_{ik},$$

and from the zeroth-order equations of $\overline{c'^2u'_i}$ (Shih 1984)

$$-\frac{1}{\rho}\overline{c'^2p'_{,i}} + \nu\,\overline{c'^2u'_{i,jj}} = \overline{u'_ju'_i}\,\overline{c'^2}_{,j} + 2\overline{u'_jc'}\,(\overline{u'_ic'})_{,j}.$$

3.2. *Third moments*

Lumley (1978*a*) constructed a form for third-moment terms from first principles. That is, these terms are not modelled in the usual sense, but are obtained by a limit process for small perturbations about a (Gaussian) equilibrium state, reminiscent of non-equilibrium thermodynamics of mixtures, where the second-order quantities (variances and fluxes) play the role of species. These model forms contain no new adjustable constants.

$$\overline{c'^2u_i} = -[\overline{c'^2_{,j}}\,\overline{u'_iu'_j} + 2(\overline{u'_ic'})_{,j}\,\overline{u'_jc'}]\,\frac{\bar{\epsilon}}{2\overline{q^2}}\Big/(r+\phi^c),$$

$$\overline{c'u'_iu'_j} = \Big\{-[(\overline{u'_ic'})_{,k}\,\overline{u'_ku'_j} + (\overline{u'_jc'})_{,k}\,\overline{u'_ku'_i} + (\overline{u'_iu'_j})_{,k}\,\overline{u'_kc'}] + \frac{\beta-2}{3}\frac{\bar{\epsilon}}{\overline{q^2}}\,\overline{q^2c'}\delta_{ij}\Big\}\frac{\overline{q^2}}{\bar{\epsilon}}\Big/(\beta+2\phi^c).$$

Modifications of these forms for the presence of the terminal velocity or the particle time constant would be of the same order as, or higher order than, the terms already neglected in the lengthscale-ratio expansion.

3.3. *Drift term*

Lottey *et al.* (1983) derived a model for the drift term from the realizability principle as follows:

$$\overline{c'_{,j}u'_i} = \overline{c'u'_i}\left\{\frac{\overline{c'^2}_{,j}}{2\overline{c'^2}} + V_{\mathrm{p}j}\frac{9\bar{\epsilon}}{\overline{q^2}\,\overline{q^2}}F_D^{\frac{1}{2}}\left[a+b\frac{(V_{\mathrm{p}i}\overline{c'u'_i})^2}{V_{\mathrm{p}i}V_{\mathrm{p}i}\overline{cu_j}\,\overline{cu_j}}\right]\right\}.$$

As discussed in detail there, this is the term that is responsible for the decrease in particle-/fluid-velocity correlation due to the crossing-trajectories effect. This effect is not embodied in (22) as might be thought, since that equation is scalar, and hence cannot distinguish horizontal from vertical. What is needed is an effect that differs in the horizontal and vertical, and that differs depending on the relative orientation of the particle flux and the gravity vector.

This term also embodies a hitherto unknown physical effect resulting from inhomogeneity (see Lottey *et al.* 1983).

3.4. *Model terms in dissipation equations*

Lumley (1978*a*) suggested

$$\overline{\epsilon' u'_j} = -\frac{3}{5}\frac{\overline{q^2}}{\bar{\epsilon}}\frac{3}{10+4\beta}\,\bar{\epsilon}_{,k}\left(\overline{u_j u_k}+\frac{2\overline{u_i u_j}\,\overline{u_k u_i}}{\overline{q^2}}\right),$$

$$\overline{\epsilon'_c u'_j} = -\frac{\overline{c'^2}}{\bar{\epsilon}_c}\frac{1}{2(1+\phi^c/r)}\,\bar{\epsilon}_{c,k}\left(\overline{u'_j u'_k}+\frac{\overline{c'u'_j}\,\overline{c'u'_k}}{\overline{c'^2}}\right)$$

and
$$\psi = \tfrac{14}{5}+0.98\exp[-2.83Re^{-\frac{1}{2}}][1-0.33\ln(1-5\mathrm{II})].$$

Shih (1984) suggested a modified model for ψ^c according to an assumption that the ratio of mechanical timescale $\overline{q^2}/\bar{\epsilon}$ to the scalar timescale $\overline{c^2}/\bar{\epsilon}$ will approach some 'equilibrium' value. The form of ψ^c is

$$\psi^c = \psi^c_0+\frac{\psi^c_1\overline{c'u'_i}\,\bar{C}_{,i}}{\bar{\epsilon}_c},$$

$$\psi^c_0 = 2-\frac{2-\psi}{r}+\frac{3}{r}(-\mathrm{II})\left(\frac{r}{r_\mathrm{e}}-1\right),$$

$$\psi^c_1 = \begin{cases} 2\left(\dfrac{r_\mathrm{e}}{r}\right)^{10} & \text{if } r < r_\mathrm{e}, \\ 2\left[1-0.1\left(1-\dfrac{r_\mathrm{e}}{r}\right)\right] & \text{if } r > r_\mathrm{e}, \end{cases}$$

where
$$\psi^c = 1+r+1.1r^2F_D^{\frac{1}{2}},$$

$$r = \frac{\overline{q^2}}{\bar{\epsilon}}\frac{\bar{\epsilon}_c}{\overline{c'^2}},$$

$$F_D \doteq 1-\frac{\overline{c'u'_i}\,\overline{c'u'_i}}{\overline{c'^2}\,\overline{u'^2_i}},$$

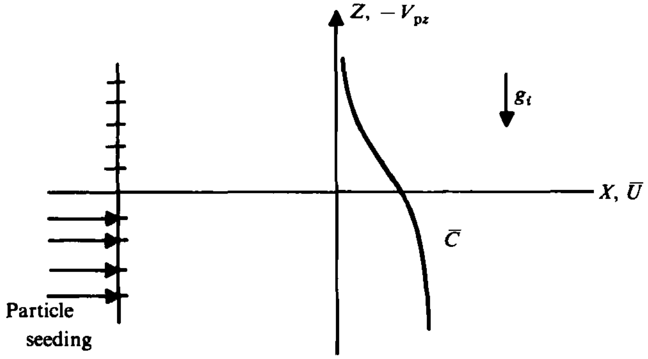

FIGURE 1. Configuration of the particle mixing layer.

$$\beta = 2+\exp[-7.77/Re^{\frac{1}{2}}]\frac{8}{Re^{\frac{1}{2}}},$$
$$a = 0.7778, \quad b = -0.725,$$
$$r_{\mathrm{e}} \doteq 2.5,$$
$$\mathrm{II} = 0 \quad \text{(isotropic turbulence)}.$$

We retain a weak Reynolds-number dependence for large but finite Reynolds number in order to match experimental data.

4. Two-dimensional mixing layer

Now let us consider the simple case of a particle mixing layer in a grid turbulence with a constant mean velocity $\bar{U}_i = (\bar{U}, 0, -V_{p3})$. The particles are seeded from the lower half-grid to form a particle mixing layer in a grid turbulent flow, see figure 1. To hold the centre of the particle mixing layer at a fixed height, we have introduced an upward fluid velocity to cancel the drift. In effect we have slightly rotated the free stream upward.

In this flow, the turbulence is isotropic, the mean density is a function of x, z: $\bar{c} = \bar{c}(x, z)$, the particle terminal velocity is $V_{pz} = \tau_p g_z$, which is a negative value. The equations for this simple case become

$$\bar{U}\frac{\partial \bar{C}}{\partial x}+\frac{\partial \overline{cw}}{\partial z} = \tau_p \frac{\partial}{\partial z}\left[-\frac{1}{\rho}\overline{cp_{,z}}+\nu\overline{cw_{,jj}}\right], \tag{24}$$

$$\bar{U}\frac{\partial \overline{c^2}}{\partial x}+2\overline{cw}\frac{\partial \bar{C}}{\partial z}+\frac{\partial \overline{c^2w}}{\partial z} = 2\tau_p\left[\frac{\partial \bar{C}}{\partial z}\left(-\frac{1}{\rho}\overline{cp_{,z}}+\nu\overline{cw_{,jj}}\right) + \frac{1}{2}\frac{\partial}{\partial z}\left(-\frac{1}{\rho}\overline{p_{,z}c^2}+\nu\overline{c^2w_{,jj}}\right)\right]-2\bar{\epsilon}_c, \tag{25}$$

$$\bar{U}\frac{\partial \overline{cw}}{\partial x}-V_{pz}\frac{\partial \overline{cw}}{\partial x}+V_{p3}\overline{c_{,z}w}+\tfrac{1}{3}\overline{q^2}\frac{\partial \bar{c}}{\partial z}+\frac{1}{3}\frac{\partial \overline{cq^2}}{\partial z} = -\frac{1}{\rho}\overline{p_{,z}c}+\nu\overline{cw_{,jj}}+\tau_p\left[-\frac{1}{3}\bar{\epsilon}\frac{\partial \bar{C}}{\partial z}\right], \tag{26}$$

$$\bar{U}\frac{\partial \overline{q^2}}{\partial x} = -2\bar{\epsilon}, \tag{27}$$

$$\bar{U}\frac{\partial \bar{\epsilon}}{\partial x} = -\frac{\bar{\epsilon}^2}{\overline{q^2}}\psi, \tag{28}$$

$$\bar{U}\frac{\partial \bar{\epsilon}_c}{\partial x}+\frac{\partial \overline{\epsilon_c w}}{\partial z} = -\frac{\bar{\epsilon}_c^2}{\overline{c^2}}\psi^c. \tag{29}$$

The models we need are listed below:

$$-\frac{1}{\rho}\overline{cp_{,z}}+\nu\overline{cw_{,jj}}=\frac{1}{5}\frac{\partial}{\partial z}\overline{cq^2}-\phi^c\overline{cw}\frac{\bar{\epsilon}}{\overline{q^2}}; \tag{30a}$$

$$-\frac{1}{\rho}\overline{c^2p_{,z}}+\nu\overline{c^2w_{,jj}}=\frac{\overline{q^2}}{3}\frac{\partial\overline{c^2}}{\partial z}+\frac{\partial(\overline{cw})^2}{\partial z}; \tag{30b}$$

$$\overline{cq^2}=-\frac{\overline{q^2}}{3}\frac{\partial\overline{cw}}{\partial z}\frac{\overline{q^2}}{\bar{\epsilon}}\Big/(1+\phi^c); \tag{30c}$$

$$\overline{c_{,z}w}=\frac{\overline{cw}}{2\overline{c^2}}\frac{\partial\overline{c^2}}{\partial z}+\overline{cw}\,V_{pz}\frac{9\bar{\epsilon}}{(\overline{q^2})^2}F_D^{\frac{1}{2}}(a+b); \tag{30d}$$

$$\overline{c^2w}=-\left(\frac{\overline{q^2}}{3}\frac{\partial\overline{c^2}}{\partial z}+\frac{\partial(\overline{cw})^2}{\partial z}\right)\frac{\overline{q^2}}{\bar{\epsilon}}\Big/2(r+\phi^c); \tag{30e}$$

where $$\phi^c=1+r+1.1r^2F_D^{\frac{1}{2}},\quad r\equiv\frac{\overline{q^2}}{\bar{\epsilon}}\frac{\bar{\epsilon}_c}{\overline{c^2}},\quad F_D^{\frac{1}{2}}=\left(1-3\frac{\overline{cw}^2}{\overline{c^2}\,\overline{q^2}}\right),$$

$$\psi=\tfrac{14}{5}+0.98\exp(-2.83Re^{\frac{1}{2}}),\quad \psi^c=2-\frac{2-\psi}{r}+\frac{C_1\overline{cw}}{\bar{\epsilon}_c}\left(\frac{\partial\bar{C}}{\partial z}\right),$$

$$C_1=\begin{cases}2\left(\dfrac{r_e}{r}\right)^{10} & \text{if } r<r_e,\\[2mm] 2\left[1-0.1\left(1-\dfrac{r_e}{r}\right)\right] & \text{if } r>r_e,\ r_e\approx 2.5.\end{cases}$$

5. Results

We have calculated a set of particle mixing layers. The particle data (listed in tables 1, 2) and the fluid-turbulence data are taken from Snyder & Lumley (1971) and Wells & Stock (1983). We will present the calculations of the distributions of the particle mean density $\bar{C}$ the intensity of density fluctuations ($\overline{c^2}$), the flux $\overline{cw}$ and $\overline{cw_p}$, the third moment $\overline{c^2w}$, the ratio of mechanical timescale to scalar timescale r (defined by $(\overline{q^2}/\bar{\epsilon})(\bar{\epsilon}_c/\overline{c^2})$), and the effective diffusivity $\gamma\equiv-\overline{cw}/(\partial\bar{C}/\partial z)$. We also calculated the differences between the density-weighted- and conventional-mean particle velocity and variances of particle-velocity fluctuations, which are defined by

$$CUPDC=\langle u_{pi}\rangle-\bar{U}_{pi},\quad CUP2DC=\langle u'^2_{pi}\rangle-\overline{u'^2_{pi}},$$

where $$\langle u_{pi}\rangle\equiv\frac{\overline{cu_{pi}}}{\bar{C}},\quad \langle u'^2_{pi}\rangle\equiv\frac{\overline{c(u_{pi}-\langle u_{pi}\rangle)^2}}{\bar{C}}.$$

Here u_{pi}, u'_{pi} are the instantaneous velocity and velocity fluctuations of the particles. Using the above definitions we may obtain

$$CUPDC=\frac{\overline{c'u'_{pi}}}{\bar{C}},\quad CUP2DC=\frac{\overline{c'u'^2_{pi}}}{\bar{C}}-\left(\frac{\overline{c'u'_{pi}}}{\bar{C}}\right)^2.$$

Using (9) we may obtain

$$CUPDC\equiv\frac{\overline{c'u'_{p3}}}{\bar{C}}=\frac{\overline{c'w'}-\tau_p\left(\dfrac{1}{5}\dfrac{\partial}{\partial z}\overline{c'q'^2}-\phi^c\overline{c'w'}\dfrac{\bar{\epsilon}}{\overline{q^2}}\right)}{\bar{C}},$$

$$CUP2DC\equiv\frac{\left(\overline{c'q'^2}-\frac{2}{3}\tau_p\overline{q^2}\dfrac{\partial\overline{c'w'}}{\partial z}\right)}{\bar{C}}-(CUPDC)^2.$$

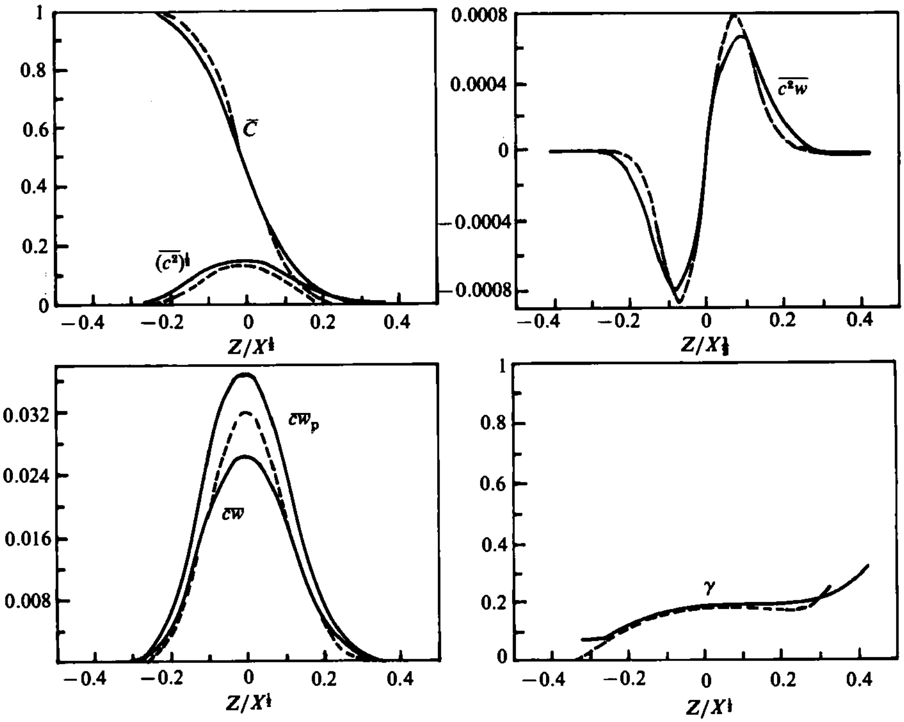

FIGURE 2. Calculated distributions of the statistical quantities: —, 57 μm glass particle with terminal velocity 23 cm/s; ---, 58 μm glass particle with same terminal velocity but zero inertia ($\tau_p = 0$).

The existing experimental data we have are from Snyder & Lumley (1971) and Wells & Stock (1983). Both of those experiments include the effect of inertia and the crossing-trajectories effect on the dispersion of particles suspended in a turbulent fluid. In a natural gravitational field, the particle motion is governed by the coupled effects of the particle inertia, the particle's free-fall velocity (crossing-trajectories effect) and the turbulent flow field. It is expected that the dispersion of light particles is controlled mainly by the turbulent flow field, but the dispersion of heavy particles should also strongly depend on inertia and the crossing-trajectories effect. The mechanism of the crossing-trajectories effect is clear: it causes heavy particles to fall from one eddy to another so that the particle-velocity autocorrelation decreases faster than it otherwise would. However, the influence of inertia is not so clear. In order to understand the individual influence of inertia and the crossing-trajectories effect on the dispersion of particles, Wells & Stock (1983) did the following experiments: the particles were charged before entry into the test section; a uniform electric field within the test section was used to suppress or strengthen the effect of gravity, making the terminal velocity zero, smaller or larger than the normal value. In this way they could isolate the individual consequences of particle inertia and the crossing-trajectories effect on the dispersion process. Their experiments are very helpful in exposing the mechanism of heavy-particle dispersion.

In our calculations, we simulated Wells & Stock's (1983) experiments by varying the terminal velocity from zero to 125 cm/s for heavy particles (57 μm glass

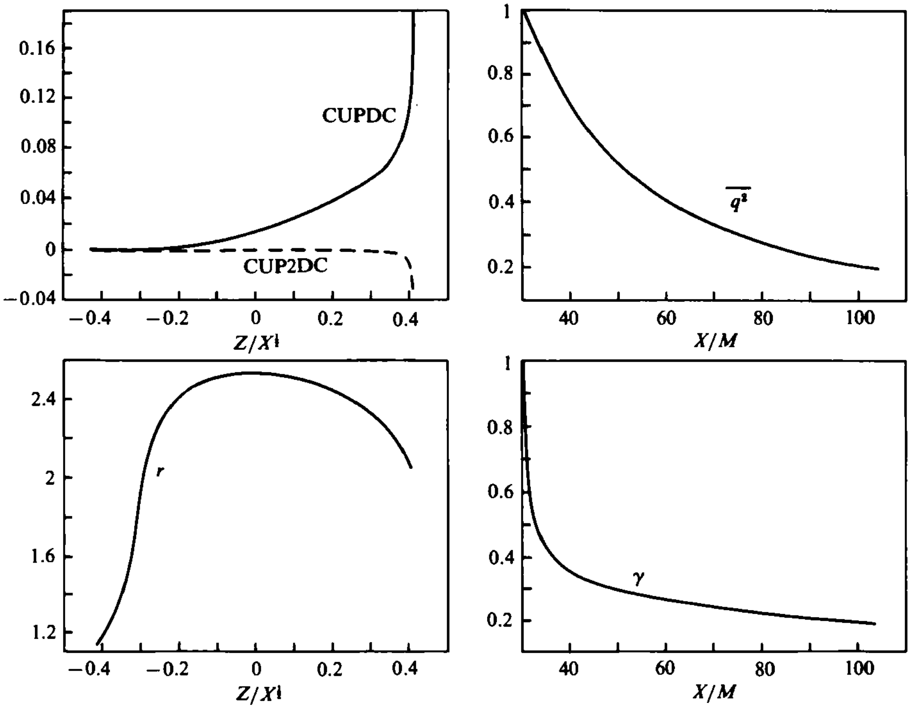

FIGURE 3. Calculated distributions of the statistical quantities for 57 μm glass particle with terminal velocity 23 cm/s.

particles), and from zero to 25 cm/s for light particles (5 μm glass particles). We also calculated cases which correspond to Snyder & Lumley's (1971) experiments (87 μm glass particles, hollow glass and corn particles).

Figures 2 and 3 are typical calculations for the 57 μm glass particles in a normal gravitational field (with terminal velocity 23 cm/s); we present the mean concentration $\overline{C}$, standard deviation of concentration fluctuation $(\overline{c^2})^{\frac{1}{2}}$, flux $\overline{cw}$, $\overline{cw_p}$, third moment $\overline{c^2w}$, effective diffusivity γ, differences of the density-weighted- and conventional-mean particle velocity and variance of particle-velocity fluctuations *CUPDC*, *CUP2DC*, and timescale ratio r crossing the particle mixing layer. All the quantities shown in the figures (except figure 4) are non-dimensional.

The development of the layer is approximately self-preserving for large times, with all lengthscales growing approximately as $X^{\frac{1}{2}}$; we have consequently plotted our profiles as functions of $Z/X^{\frac{1}{2}}$.

In figure 3, the evolution of turbulent energy and effective diffusivity are also presented. To see the influence of inertia, we also present in figure 2 calculations in which we set inertia to zero (i.e. $\tau_p = 0$). From these figures, we see that the inertia of the particles increases the fluctuations of particle concentration $\overline{c^2}$. Clearly an initially uniform distribution of particles with inertia in a non-uniform velocity field would develop non-uniformities of concentration. We can also see that the flux $\overline{cw}$ and $\partial \overline{C}/\partial z$ are both decreased by the inertia of the particles. This means that the effective diffusivity (the ratio of these two) will not be significantly changed by the particle inertia. This matches the asymptotic theory (Csanady 1963) that the effective diffusivity of the particles is independent of particle inertia. In this

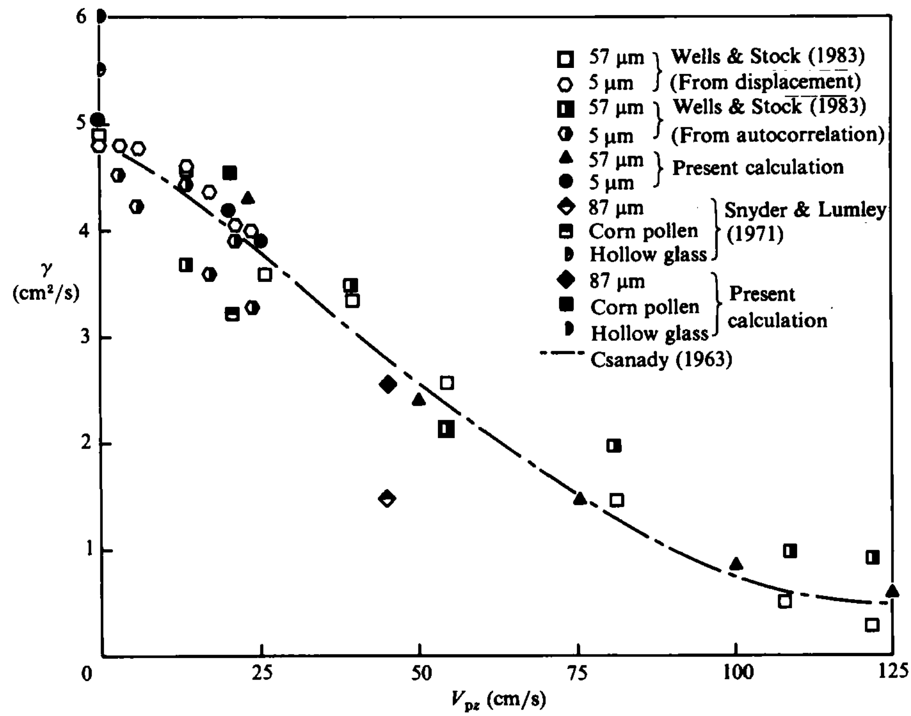

FIGURE 4. Comparison of the diffusivity calculated at the middle of mixing layer with experiment.

particular calculation, the inertia of the particles increased the diffusivity by less than 5%.

The shape of the effective diffusivity profile γ deserves some explanation. Lumley pointed out that the diffusivity would be increased in the lower part and decreased in the upper part by the influx of the variance of concentration, which has a different gradient in the upper and lower part of the mixing layer (Lottey *et al.* 1983). Here the situation is different because there is a mean-velocity component $w = -V_{pz}$; hence the second term in the flux equations, $w\,\partial\overline{cw}/\partial z$, will over-balance the third term $\overline{C}_{,z}\,V_{pz}$ which contains the influence of the influx of concentration. Our calculations show that the diffusivity is higher in the upper part and lower in the lower part.

To see the influence of the crossing-trajectories effect, we calculate the heavy (57 µm glass) particles with terminal velocities of 50 cm/s, 75 cm/s, 100 cm/s and 125 cm/s and the light particles (5 µm glass) with terminal velocities 0.188 cm/s, 20 cm/s and 25 cm/s. The profiles of all quantities are quite similar to the profiles in figures 2 and 3. From these calculations, we see that the main influence of the crossing-trajectories effect is to decrease the particle dispersion and related quantities.

We also calculated the particles (hollow glass, 87 µm glass and corn pollen) which correspond to Snyder & Lumley's (1971) experiments.

Figure 4 is the comparison with experiment of the diffusivity of all particles calculated at the middle of the mixing layer. The calculated value of diffusivity is taken at $X/M = 90$ for comparing with Wells & Stock's data and at $X/M = 210$ for Snyder & Lumley's data. Figure 4 shows that the diffusivity from different measurements (particle displacement and autocorrelation) are quite scattered. However, our calculations are in reasonable agreement with experimental data.

Note that the curve obtained from Csanady (1963) does an excellent job. Our second-order model would be unnecessary if Csanady's parametrization could be applied everywhere. However, this simple parametrization (for a discussion see Lumley 1978*c*) is restricted to long times and homogeneous situations. The purpose of developing our elaborate second-order model, which we are here calibrating in an essentially homogeneous situation (at least insofar as the velocity field is concerned), and for large times, is that it can be applied in inhomogeneous, unsteady, more practical situations, unlike the Csanady parametrization.

Finally, from figure 3 we may notice that the difference of density-weighted and conventional particle mean velocity is quite significant in the lower-density region. This essentially reflects the fact that particles finding themselves far from the centre of the mixing layer (in the low-density region) must have been travelling faster than average. This is important for measurements with the laser-Doppler anemometer, as we expect that the presence or absence of particles at the measuring point (severe in the lower density region) will introduce a considerable bias in the measured velocity.

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