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A Trajectory-Simulation Model for Heavy Particle Motion in Turbulent Flow

For many purposes it is useful to be able to mimic the paths of heavy particles in a turbulent flow. This paper gives a simple procedure by which this may be achieved, provided particle spin is not important and under the restriction that the ratio of particle to fluid density exceeds about 1000. The procedure is related to the models of Faeth (1986) and Hunt and Nalpanis (1985). Simulation of the experiments of Snyder and Lumley (1971) yielded acceptable agreement with the observed rate of heavy particle dispersion.

1 Introduction

In this paper we present a new method for the simulation of heavy particle trajectories in a turbulent flow. The method could be applied to calculate, for example, the drift of aerial spray or the distribution of fuel droplets within a combustion chamber (please note, however, that to date the method has been tested against observations only for the case of nearly homogeneous turbulence). The superiority of the Lagrangian approach to turbulent dispersion has been evident since it was developed by Taylor (1921). With the advent of accessible computing power it has become possible to mimic turbulent dispersion by calculating a large number of random trajectories from the source to the point of interest. This is the Lagrangian stochastic (or trajectory-simulation) method.

The fundamental advantage of the Lagrangian approach is that it correctly predicts the rate of dispersion in the near field of a source, whereas all attempts to close the heirarchy of Eulerian conservation equations have yielded solutions which are seriously in error close to the source. Thus if first-order closure (K-theory) is adopted, the eddy diffusivity (K) can be shown to depend not only upon the characteristics of the turbulence but also upon the time of travel (or distance) from the source. (Csanady, 1973; Batchelor, 1949).

Correct treatment of the near field is crucial in simulation of turbulent transport within crops or forests, and the adaptation of the Lagrangian stochastic method to this type of problem has lead to rapid development of supporting theory (see Durbin, 1983; van Dop et al., 1985; Thomson, 1984 and 1987; Sawford, 1986; Pope, 1987; Sawford and Guest, 1988). While some fundamental problems remain it is well established (e.g., Wilson et al., 1981) that the trajectory-simulation method can give accurate predictions for complex dispersion problems given only a crude knowledge of the flow field—the mean velocity, the velocity-fluctuation variances, and the autocorrelation timescale.

In the case of heavy particle dispersion, the trajectory-simulation method has a further advantage over other methods in that it is easy to include time-dependent processes such as droplet size reduction due to evaporation. However it is more difficult to calculate a heavy particle path than a fluid element path, because the velocity sequence driving the heavy particle is neither a fluid Lagrangian nor an Eulerian sequence. Therefore one must encapsulate both the temporal and the spatial correlation of the fluid velocity field rather than just the Lagrangian temporal correlation.

There are two approaches to the calculation of heavy particle trajectories. The first option is to calculate both the particle velocity u_{pi} and the fluid velocity u_i in the immediate vicinity of the particle, these velocities being linked by the equation of motion of the particle. The core of the problem then lies in determination of the fluid forcing velocity u_i. The work by Hunt and Nalpanis (1985) and Faeth (1986) falls into this category, as does the model we present. The alternative option is to establish the heavy particle velocity statistics (velocity variance and autocorrelation timescale). Given these statistics one may apply Taylor's analytical result, or, in the case of inhomogeneous turbulence, carry out a trajectory simulation. The recent work by Walklate (1987; see also comments by Wilson and Zhuang, 1988) belongs to this category.

Section 2 describes the new model, and section (3) presents simulations of the heavy particle dispersion experiments of Snyder and Lumley (1971).

2 Formulation of New Model

Provided the ratio ρ_p/ρ of particle density to fluid density is large ($>10^3$) the equation of motion for a rigid nonrotating spherical particle may be written (Schlicting 1968, Hjelmfelt and Mockros 1966):

$$du_{pi}/dt = F(u_i - u_{pi}) - g_i \tag{1}$$

Here the total instantaneous fluid velocity $u_i(t)$ may be decomposed into a mean and fluctuation $u_i(t) = U_i + u_i'(t)$, and g_i is the gravitational acceleration vector. F, whose reciprocal is the particle acceleration timescale, is given by:

$$F = (3/4)\ C_d\ \rho/\ (d\rho_p)\ |u_i - u_{pi}| \tag{2}$$

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where d is the particle diameter and C_d is a drag coefficient

$$C_d = 24(1 + 3R_e/16)/R_e \tag{3}$$

Equation (1) is valid only for $R_e \lesssim 5$, where R_e is the slip Reynolds number:

$$R_e = d\,|u_i - u_{pi}|/\nu \tag{4}$$

Here ν is the kinematic viscosity of the fluid. Equation (1) is a nonlinear stochastic equation which may be integrated numerically to determine the heavy particle trajectory provided one can determine an appropriate (stochastic) sequence of values for the driving fluid velocity at discrete times $t^{(k)}$.

In our model, as in that of Faeth (1986), the driving fluid velocity undergoes abrupt, random changes as the particle encounters new eddies. Between these changes, while the particle passes through a given eddy, the driving fluid velocity remains correlated along the particle path but not, as in Faeth's model, constant.

When the particle encounters a new eddy we mark as the "star" the fluid element surrounding the particle at that instant (see Fig. 1). The particle is considered to stay within the present eddy until its separation from the star exceeds a chosen lengthscale L. To monitor this separation R, i.e., the passage from one eddy to the next, we calculate the trajectories of both the particle and the star.

We need correlated time series for the star velocity u_{*i}' and the driving fluid element velocity u_i'. These we generate using the Markov chains:

$$q_{*i}^{(k+1)} = \alpha_{*i} q_{*i}^{(k)} + \mu_{*i}^{(k+1)} \tag{5a}$$

$$q_i^{(k+1)} = \alpha_i q_i^{(k)} + \mu_i^{(k+1)} \tag{5b}$$

where the q's are dimensionless quantities which are scaled to obtain the velocity fluctuations

$$u_{*i}'^{(k)} = \sigma_i q_{*i}^{(k)} \tag{6a}$$

$$u_i'^{(k)} = \sigma_i q_i^{(k)} \tag{6b}$$

The summation convention does not apply in equations (5, 6) and σ_i is the velocity standard deviation. In the Markov chain equations (5a, b) the α's control the correlation between consecutive values of the velocity fluctuation. The μ's are random variations. To ensure unit variance for the q's the μ's must have the form

$$\mu^{(k)} = \sqrt{1-\alpha^2}\;\gamma^{(k)} \tag{7}$$

where the γ's are random numbers having zero mean and unit variance. $\gamma_1^{(k)}$, $\gamma_2^{(k)}$, and $\gamma_3^{(k)}$ are independent of each other and of their values at any other time.

Each time the heavy particle encounters a new eddy and a new star is marked, say at time $t^{(0)}$, the Markov chains are reset

$$q_{*i}^{(0)} = q_i^{(0)} = \gamma_i^{(0)} \tag{8}$$

so that at that instant the driving fluid element and the star, being coincident, have equal velocities. The total velocities are obtained from the fluctuations by adding the mean. It remains to specify the α's.

For the star trajectories we require a fluid Lagrangian series, and the choice

$$\alpha_{*i} = \exp[-\Delta t/T_L] \tag{9a}$$

is conventional; here T_L is the Lagrangian integral timescale.

In the case of the time series for the driving fluid velocity we use the simple expression

$$\alpha_i = \exp[-\Delta t/T_L - |\Delta r_i|/L_g] \tag{9b}$$

where L_g is the lateral integral lengthscale and Δr_i is the separation between the previous and the present driving fluid element, i.e., the separation between the driving fluid element at the previous time $t^{(k)}$ and at the present time $t^{(k+1)}$. The reasoning behind equation (9b) is simple. Figure 1 identifies

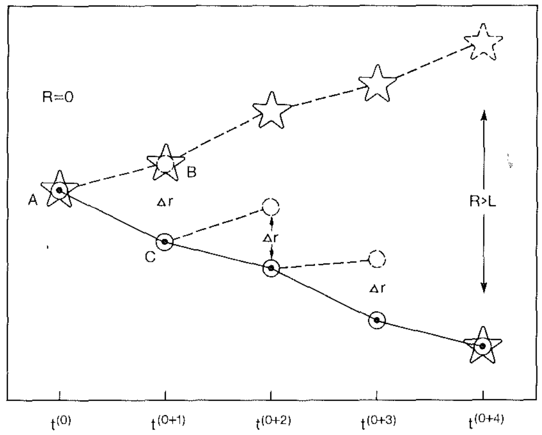

Fig. 1 Defining sketch for trajectory calculations showing the discretized path of a heavy particle (●) which is slipping downwards relative to the fluid around it. For clarity motion is shown only in the vertical direction. At each location (○) denotes the driving fluid element and (☆) the "star," a special fluid element identifying the eddy within which the particle now lies. A dashed image (○, ☆) implies that the element is not tracked beyond its present location. R is the separation between the particle and the star, and Δr is the separation between the particle and that fluid element which, at the previous time, was the driving fluid element.
At time $t^{(0)}$ the particle has entered a new eddy and the star is marked. At $t^{(0+1)}$ $\Delta r = R < L$, where L is the eddy lengthscale. At $t^{(0+2)}$ and $t^{(0+3)}$ $\Delta r < R < L$. At $t^{(0+4)}$ the particle has departed the eddy, i.e., $R > L$, and entered a new one. The new star is marked.

the heavy particle and the star, both at the location A at the instant the particle enters a new eddy. In the succeeding timestep Δt the star moves to B and the heavy particle to C. Provided the separation R between the particle and the star does not exceed the lengthscale L we consider the driving fluid velocity to be correlated with its previous value. We specify the correlation coefficient over interval Δt to be the product of the Lagrangian correlation coefficient along the (previous driving element) path AB and the Eulerian spatial correlation coefficient for the separation BC between the previous and the new driving element.

The timestep has been specified as

$$\Delta t = 0.1 \text{ minimum } (\tau_p, T_L) \tag{10}$$

where τ_p is the particle time constant. A discussion of the choice of the timestep for Lagrangian stochastic models is given by Wilson and Zhuang (1989). Our criterion (10) ensures that the choice of a smaller timestep will not affect the outcome of a simulation. Earlier simulations by Hunt and Nalpanis (1985) did not in all cases satisfy this necessary limitation on the timestep and may have yielded simulations whose agreement with experiment is misleading. The lengthscale L has been specified as

$$L = CL_g \tag{11}$$

A single value for C is to be used for all particle sizes. We found that the specification $C = 1.5$ gave best agreement with the Snyder and Lumley data.

Our model differs from that of Faeth (1986) primarily in our treatment of the driving fluid velocity as varying within each eddy. In Faeth's model the driving velocity was constant within an eddy and changed randomly (without correlation) when either the separation between the particle and the (constant-velocity) star exceeded a specified lengthscale or when a specified time had elapsed since the last fluid velocity choice. Faeth had available two adjustable constants and indicated that the model yielded simulations in good agreement with the Snyder and Lumley data.

3 Comparison With Observations

Snyder and Lumley (1971; hereafter SL) measured the

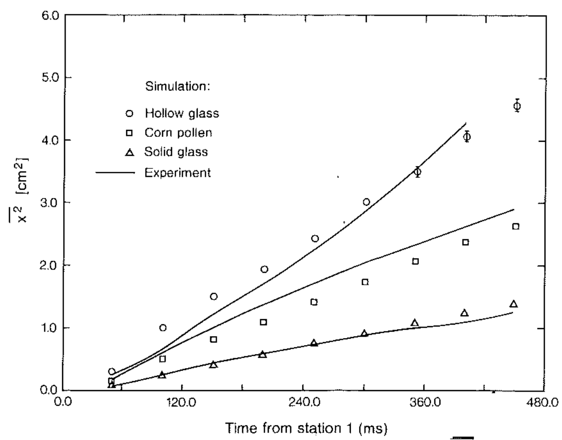

Fig. 2 Mean square heavy particle displacement $\overline{x^2}$ in the cross-stream direction as a function of time. Comparison of simulations with the experimental data of Snyder and Lumley (1971). Symbols give model solutions for:
- ○ **Hollow glass $\tau_p = 1.7$ millis.**
- □ **Corn pollen $\tau_p = 20.0$ millis.**
- △ **Solid glass $\tau_p = 45.0$ millis.**

Error bars give +/− the standard error of the mean.

dispersion of several types of particles which were injected into the decaying turbulence downstream from a grid in a wind tunnel. In addition to the particle dispersion data, comprehensive fluid velocity statistics were measured. The mean stream direction (x_3) was vertical. In our simulation we have included the variation of the velocity statistics along the stream. The streamwise and cross-stream fluid velocity variances are given by SL equations (9, 10). In decaying grid turbulence the timescale is expected to vary linearly with the streamwise coordinate, and from SL Fig. 14 we inferred that:

$$T_L = 0.1(x_3/M - 14)/(73 - 14) \tag{12}$$

where $M = 0.0254$m is the grid mesh length and $x_3/M = 14$ is our choice for the virtual origin of the decay. The transverse lengthscale was specified as:

$$L_g = T_L/\sigma \tag{13}$$

where σ is the transverse velocity standard deviation.

Density ratios ρ_p/ρ for the particles released by SL ranged from 8900 for solid glass down to 260 for hollow glass. The value $\rho_p/\rho = 260$ for hollow glass violates the restriction $\rho_p/\rho > 1000$ placed on the particle equation of motion (1). However if we estimate a typical value of the Stokes number

$$N_s = \sqrt{\nu/2\pi f d^2} \tag{14}$$

by setting the frequency $f = 1/T_L$ we obtain, for the hollow glass beads of the SL experiment, $N_s \sim 10$. At such a value for N_s (and even at values corresponding to a tenfold increase in frequency) it can be shown (Hjelmfelt and Mockros, 1966) that equation (1) is a very good approximation.

For each particle type released by SL we performed 10 simulations, in each of which we calculated 200 trajectories on an IBM PC-AT. Calculation of 2000 trajectories took approximately 2 hours using a "C" language program. During the simulations the slip Reynolds number was monitored. For the lightest particles, hollow glass ($\rho_p/\rho = 260$), R_e averaged 0.2. For the solid glass particles ($\rho_p/\rho = 8900$), R_e averaged 2.5.

Figure 2 shows the observed and calculated values for the mean-square transverse particle displacement as a function of time. The error bars shown +/− one standard error. The agreement between the observed and simulated spread is satisfactory.

4 Conclusion

We believe our model to be an improvement over earlier work. The temporal variation of the driving velocity is more realistic (we think) than is the case for Faeth's (1986) model; furthermore our model contains only 1 optimisable constant. We obtained a satisfactory simulation of the spread of Snyder and Lumley's lightest particles using an appropriate value for the timestep, whereas we believe the timestep used by Hunt and Nalpanis (1985) was unjustifiably large.

The generality of our method is limited by neglect of particle spin and other terms in the equation of motion. At one extreme, particles which are both small ($d <$ Kolmogorov lengthscale) and light ($\rho_p \leq \rho$) can legitimately be treated as fluid elements. At the other extreme, a small and very massive particle, our model is limited only by the restriction on the slip Reynolds number and an alternative formulation of the acceleration timescale (1/F) could be substituted.

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