Role of Turbulent Shear Stresses in Particle Dispersion

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Nomenclature

C_D = drag coefficient
d_P = particle diameter
g = gravitational acceleration
Re = Reynolds number
t = time
v = gas velocity
v_P = particle velocity
x = position
ρ = gas density
ρ_P = particle density

Introduction

THE technological applications of combustion processes in many cases involve the use of two phase flows or sprays. A large number of other important industrial and physical processes make use of turbulent two phase flows. The calculation of these flows is not at all trivial, particularly if the sprays are dense and the turbulence is modulated by the particle phase. Several methods have been developed for the calculation of these flows.[1] If the two phases are treated separately, then the stochastic simulation technique[2,3] has considerable attraction for the modeling of practical spray systems.

In the stochastic simulation method a turbulence closure model is used to develop an Eulerian description of the turbulent flowfield. Statistics of the velocities at a single point in the flow are obtained from this calculation; these statistics include the means and the variances of the velocity components. If a Gaussian probability distribution function (PDF) for the velocity is assumed, in reasonable accord with available measurements, then a random number generator may be used to sample the PDF. With these velocity samples the position of particles may be advanced by integrating the particle equation of motion through the flowfield. The equation of motion is, in most cases, simply the equation for the rate of change of momentum due to the drag operating on the particle. In the case of a fluid particle, the motion is obtained by simply integrating the particle velocity to obtain updated particle positions.

Many authors[2,3] have assumed that turbulent shear stresses do not play a role in the dispersion of particles in their stochastic simulations. However, there is no a priori justification for the omission of the shear stresses from stochastic, Lagrangian simulations of the type that have been discussed so far. Berlemont et al.[4] have developed the most complete formulation of the particle dispersion problem, wherein they used a mathematical process to impose the correct correlations between the fluid velocity components. The correlations or turbulent shear stresses were obtained from an algebraic closure model. In addition, their approach was extended to include a realistic autocorrelation function for fluid velocity in contrast to the older methods of Shuen et al.,[3] who assumed that the fluid velocity was perfectly correlated for the lifetime of an eddy or for the particle transit time across an eddy. Berlemont et al.[4] applied their model to isothermal jet flows, but they did not report the importance of the role of the turbulent shear stresses in the dispersion phenomenon.

The role of shear stresses or, equivalently, the correlation of velocity components has not been evaluated explicitly in a stochastic dispersion model. Lee and Dukler[5] extended the early work of Corrsin (reported in Lee and Dukler[5]) to examine the role of the turbulent shear stresses on fluid particle dispersion in a uniform shear flow. They used an analog computer with both uncorrelated and correlated white noise to simulate turbulence. Their results showed partial verification of Corrsin's theory in that the shear stresses did not have an impact at early times of flight of the particles or at long times but there was some impact at intermediate times. The magnitude of the effect was a function of the velocity gradient in the flow. However, their results are not directly applicable to a turbulent jet.

The purpose of this short Note is to test the role that velocity correlations or the turbulent shear stresses play in a stochastic simulation of particle dispersion in a jet. A conventional Lagrangian stochastic simulation of particle motion has been applied in conjunction with a second-order Eulerian closure model for a turbulent jet. The shear stresses have been introduced by correlating the axial and radial velocity components in an appropriate manner.

Calculations

The Eulerian flowfield for a turbulent, round jet of air was calculated with the Reynolds stress model of Farshchi et al.[6] This model has been validated extensively in isothermal and reacting flows and has been shown to yield accurate results for the turbulent shear stresses. The exit velocity of the air was 60 ms^{-1}, giving a Reynolds number of 40,000.

The dispersion of hexadecane particles in this flowfield was simulated with a Lagrangian calculation in the manner described by Shuen et al.[3] The particle position was tracked by integrating the particle equations of motion; the procedure was repeated for 2000 particles to give adequate statistics. The only forces that were presumed to act on the particles were the drag and gravitational forces; Bassett and other forces were not likely to be important for the large particle-to-gas density ratio that was considered. A balance of forces acting on the particles yields the following equation:

$$\frac{\mathrm{d}\bar{v}_P}{\mathrm{d}t} = 3\rho C_D \frac{|\bar{v} - \bar{v}_P|(\bar{v} - \bar{v}_P)}{4 d_P \rho_P} + \bar{g} \tag{1}$$

in which the drag coefficient C_D is

$$C_D = \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right), \qquad Re \le 1000 \tag{2}$$

and the velocities of the particles are given by

$$\frac{\mathrm{d}\bar{x}_P}{\mathrm{d}t} = \bar{v}_P \tag{3}$$

The equations are integrated through the flowfield with a fourth-order Runge-Kutta scheme.

The velocity vector that appears in these equations is obtained from sampling the statistical distributions of the local velocity components. A random number generator is used to sample the Gaussian PDF. These velocity samples have a mean and variance consistent with the results of the turbulence model. If a k-ϵ turbulence model is used, then the three velocity components are generally assumed to be uncorrelated, i.e., the shear stresses are not reflected in the statistical sam-

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ples of the gas phase velocities. Other turbulence models can supply this information directly as part of the calculation.[4]

The Reynolds stress code provides accurate values for the turbulent shear stresses from which the correlations between the velocity components can be calculated in a straightforward manner. This information is then used to impose a correlation on the randomly sampled velocities. We have developed the following procedure. At a given location in the flowfield, the correlation between the axial and the radial velocity is obtained from the Reynolds stress closure model. The eigenvalues of the turbulent stress tensor are determined, and these values are used to rotate the original coordinate frame into the principal axes in which the shear stresses are zero, i.e., the correlations between velocity components are zero. The velocity PDFs are sampled in this coordinate system. The velocities obtained are rotated back into the original coordinate frame in which the correct correlation between velocity components is now imposed. Particle positions are advanced by integration with these velocities. The statistics of the randomly generated velocities have been checked to ensure that the appropriate correlations are obtained. By this means we can generate a velocity field that reproduces not only the mean and variances of the true velocity field but also the turbulent shear stresses.

Particles are tracked as they move through the simulated flowfield. Because this is a Lagrangian simulation, the primary independent variable is the particle time of flight. An important aspect of the procedure is the specification of the time for a particle to interact with an eddy. The procedure of Shuen et al.[3] has been followed. It is also possible to monitor the particle position and velocities as they pass through a particular plane of the jet. Thus, it is possible to present Eulerian statistics that can be more useful in terms of comparisons with measurements.

Results and Discussion

The dispersion $D_R(t_f)$ is defined as the mean square displacement of the particles from the centerline of the jet on which they were released, i.e.,

$$D_R(t_f) = \frac{\sum_{j=1}^{N} [r_j(t_f) - r_j(0)]^2}{N} \tag{4}$$

in which t_f is the particle time of flight, r_j is the radial location of the jth particle, and N is the total number of particles considered. Two sets of calculations were performed. In one case, the correlations between the sampled velocities were zero, i.e., the Reynolds stresses were neglected in the simulation of particle dispersion. In the other case, the results of the Reynolds stress model were used to sample the velocity PDFs with the correct correlation between components.

The dispersion of fluid particles, i.e., particles with zero mass, is presented in Table 1. The calculated dispersion of 100 μm diam droplets of hexadecane is presented in Table 2. It is worth noting that the early time behavior of the dispersion appears to be a quadratic function of time, which is expected from theory for any finite velocity.[7] At later times the dispersion appears to increase linearly, which is also expected for a self-preserving round jet.[7] Reasonably good agreement between the stochastic simulation without the shear stress correlation and experiments has been demonstrated in an earlier study.[8]

The results show that the turbulent shear stresses play little or no role in the simulation of the dispersion of both discrete and fluid particles. It has, of course, been customary to neglect these terms in the usual stochastic models of particle dispersion, and this assumption is validated by the present results for discrete particles. However, the fact that the turbulent shear stresses play almost no role in determining the rate of dispersion of fluid particles may appear surprising. It is precisely these terms and analogous covariances that account for the transport of momentum and scalars in the turbulent jet. The stochastic simulation approach does not admit a direct role for the shear stresses. Rather, they influence events mostly through the generation of turbulent kinetic energy, which, in turn, leads to larger variances for the velocity field.

Table 1 Dispersion of fluid particles

Times of flight from nozzle, ms	Dispersion without velocity correlation, mm^2	Dispersion with velocity correlation, mm^2
2	6.85	6.66
5	61.9	60.7
10	155	152
15	254	250
20	351	345
30	550	538
40	730	737
60	921	929

Table 2 Dispersion of 100 μm hexadecane particles

Times of flight from nozzle, ms	Dispersion without velocity correlation, mm^2	Dispersion with velocity correlation, mm^2
2	0.005	0.005
5	0.774	0.786
10	5.94	5.87
15	14.5	14.3
20	25.5	25.2
30	53.5	53.0
40	90.4	89.1
60	200	194

Conclusions

It has been shown that a stochastic simulation of particle dispersion in a turbulent shear flow can be modified to incorporate the effect of turbulent shear stresses or correlations of the random velocity fluctuations that are imposed on a particle. However, the correlation of velocity components had a negligible impact on the rate of dispersion of particles, whether they were large, discrete particles or fluid particles without inertia.

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