Simulation of Dispersion of Heavy Particles in Confined Turbulent Flows

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The turbulent dispersion of particles is of major importance in such diverse applications as liquid fuel and coal combustion, reaction quenching in (for example) petroleum chemistry, sediment transport in rivers and gas-solid separation in cyclones. In recent years there has been increased emphasis on the development of mathematical models to predict the behavior of particles and/or droplets in turbulent flows and these can be grouped under the two categories of Eulerian and Lagrangian methods. In the Eulerian approach (Gibson and Morgan, 1970) a conservation equation for the mass fraction of particles is derived and solved along with the governing equations of fluid motion under the assumption that the particles move with the gas. Although the problem of inequality of the diffusion coefficients of fluid parcels and heavy particles has recently been addressed (Berlemont and Gouesbet, 1982), the no-slip approximation has been retained. In the Lagrangian approach a representative number of individual particle trajectories are calculated within the Eulerian gas flow field, which is obtained either experimentally or through the solution of the governing equations of the gas phase complemented by a suitable turbulence model (Sumer, 1973; Gosman, 1981). The results of the large number of particle trajectory calculations are ensemble averaged to give the particle concentration distribution defined in the Eulerian sense.

This paper describes the application of a Lagrangian formulation to experimental situations both in pulverized coal burners reported by Thurgood et al. (1980) and the case of particle-laden cold flow of Tice and Smoot (1978) to validate the physical modelling.

NUMERICAL SIMULATION

When all external forces except for the drag force are neglected, the equations of motion of a small particle in a gaseous environment can be expressed in a Lagrangian frame of reference as

$$du_p/dt = -\propto (u_p - \tilde{u}) \tag{1}$$

$$dv_p/dt = -\propto (v_p - \tilde{v}) + w_p^2/r_p \tag{2}$$

$$dw_p/dt = -\propto (w_p - \tilde{w}) - v_p w_p/r_p \tag{3}$$

$$\propto = (18\mu/\rho_p D_p^2)(C_D Re/24) \tag{4}$$

where u_p, v_p, w_p and $\tilde{u}$, $\tilde{v}$, $\tilde{w}$ are the instantaneous components of the particle and gas velocities respectively in the x, r and θ directions of a cylindrical polar system of coordinates.

These equations are supplemented by the following which describe the instantaneous location of the particle

$$dx_p/d\zeta_p = u_p, \quad dr_p/dt = v_p, \quad d\theta/dt = w_p/r_p \tag{5}$$

where x_p, r_p and θ_p are the space co-ordinates.

The drag coefficient C_D is expressed as a function of the relative Reynolds number with the general form

$$C_D = a_1 + a_2/Re + a_3/Re^2 \tag{6}$$

where the a's are given for several ranges of Reynolds number by Morsi and Alexander (1972) so that Stokes regime is obeyed for $Re < 0.1$ and for $0.1 < Re < 1.0$ the a's taking the value 3.69, 22.73 and 0.0903 respectively.

To account for the effects of turbulence on the trajectories of individual particles the instantaneous gas velocity $\tilde{u}$ is decomposed into time-mean and fluctuating components $\overline{u_i}$ and u_i'. It is assumed that the fluctuating velocity prevails, on average, for a time period equal to the life time of the fluid eddy that the particle is traversing, which can be expressed in terms of the local kinetic energy of turbulence, k, and its dissipation rate ϵ as (Hinze, 1975).

$$\tau \cong 0.16 \frac{k}{\epsilon} \tag{7}$$

The values of the fluctuating velocities can be assumed to possess a Gaussian distribution so that these are related to the root mean square fluctuations by

$$u_i' = \phi\,(u_i^2)^{1/2} \cong \phi\,(\overline{u^2})^{1/2} \tag{8}$$

where ϕ is a normally distributed random variable and u_i' represents the fluctuating components of velocity in the r, x and θ directions, the overbar indicating time averaging.

SOLUTION PROCEDURE

The information required to carry out the simulation described above, namely the local values of the flow variables and turbulence quantities have been obtained from the solution of the governing equations of conservation of mass and momentum in the gas phase. These equations can be expressed for brevity in Cartesian tensor notation as

$$\frac{\partial}{\partial x_j} \rho u_j = 0 \tag{9}$$

$$\frac{\partial}{\partial x_j} \rho u_j u_i = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu_{\text{eff}} \frac{\partial u_i}{\partial x_j}\right) + F_i \tag{10}$$

where p is the pressure, ρ the gas density and μ_{eff} the effective viscosity which is the sum of laminar and turbulent viscosities, μ and μ_t. Here, F_i stands for the momentum sources or sinks arising from the interaction between the gas and the solid particles. Turbulence is modelled by the widely used k-ϵ model which entails the solution of a transport equation for the kinetic energy of turbulence k and another for its dissipation rate ϵ, which are given by

$$\frac{\partial}{\partial x_j} \rho u_j k = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j}\right) + \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \frac{\partial u_i}{\partial x_j} - \rho\epsilon \tag{11}$$

$$\frac{\partial}{\partial x_j} \rho u_j \epsilon = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j}\right) + C_1 \mu_t \times \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \frac{\partial u_i}{\partial x_j} \frac{\epsilon}{k} - C_2 \rho \frac{\epsilon^2}{k} \tag{12}$$

and the turbulence viscosity μ_t is obtained from

$$\mu_t = C_\mu \rho \frac{k^2}{\epsilon}, \tag{13}$$

where C_1, C_2, C_μ, σ_k and σ_ϵ are constants which are given the values $C_1 = 1.44$, $C_2 = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1$ and $\sigma_\epsilon = 1.3$.

The above set of partial differential equations (Eqs. 9–12) have been reduced into algebraic form by integration over the finite volumes into which the solution domain is subdivided. The velocity components and pressure at each control volume are calculated, using the SIMPLE algorithm (Patankar, 1980), iteratively on a digital computer.

Once the details of the flow field are known, it is possible to perform the particle trajectory calculations by integrating the equations of motion. Using a sampled value of the fluctuating gas velocity, as defined in Eq. 7, treating the body force terms in Eqs. 2 and 3 as constant over a short time interval, we can obtain closed form expressions for u_p, v_p and w_p as follows:

$$u_p = \bar{u} + u' + (u_{p,o} - \bar{u} - u')\exp[-\alpha(t - t_o)] \quad (14)$$

$$v_p = \bar{v} + v' + \frac{w_{p,o}^2}{\alpha r_{p,o}} + \left(v_{p,o} - \bar{v} - v' - \frac{w_p^2}{\alpha r_{p,o}}\right)\exp[\alpha(t - t_o)] \quad (15)$$

$$w_p = \bar{w} + w' - \frac{w_{p,o}v_{p,o}}{\alpha r_{p,o}} + \left(w_{p,o} - \bar{w} - w' + \frac{V_{p,o}w_{p,o}}{\alpha r_{p,o}}\right)\exp[-\alpha(t - t_o)] \quad (16)$$

where the subscript o pertains to the conditions at the beginning of the time step. The location of the partial is obtained by simple stepwise integration of the equations of trajectory (Eq. 5).

The calculation of a large number of particle trajectories yields the distribution of particles, and thus particle concentration, throughout the domain of interest.

RESULTS AND DISCUSSION

Comparisons have been made with published experimental results for particle mass fluxes by simulating an isokinetic sampling probe during the computational run. The stochastic nature of this technique is responsible for the scatter in the computed points.

Figure 1 is a comparison between computations and the experimental results of Tice and Smoot (1978) for a 0.2 m diameter mixing chamber into which silicon powder of 54.1 μm mean diameter was injected in lieu of coal, so that the experiment was isothermal. The experiment is described in Tice and Smooth (1978) as test 4b.

Figure 2 shows comparison between a reacting flow case reported by Thurgood et al. (1980) as "Condition A" for a 0.2 m diameter vertical combustion chamber and isothermal flow numerical test. The shape of the experimental curve is well reproduced even by nonreacting simulation. It must be pointed out that no effort was made to extend the numerical experiment beyond normalized axial locations larger than 100, to avoid complications

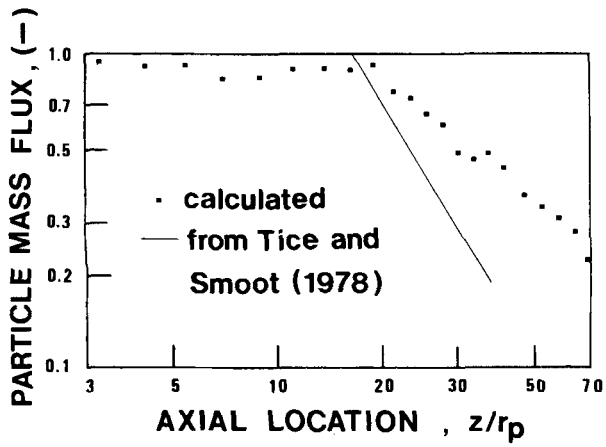

Figure 1. Axial profiles of normalised particle mass flux.

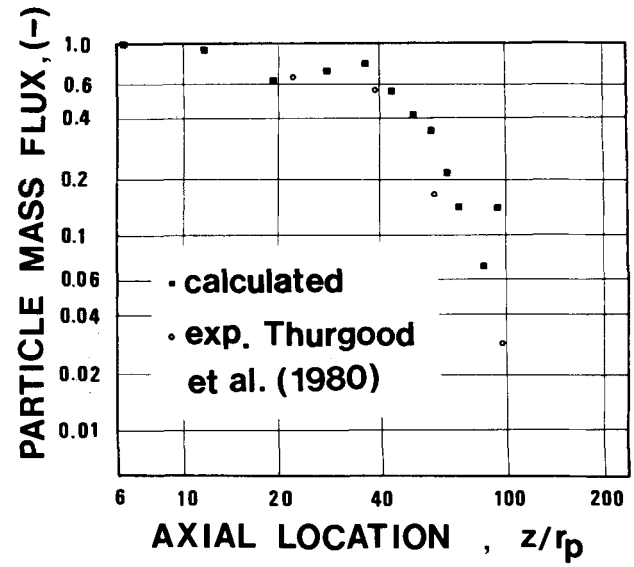

Figure 2. Axial particle dispersion profiles.

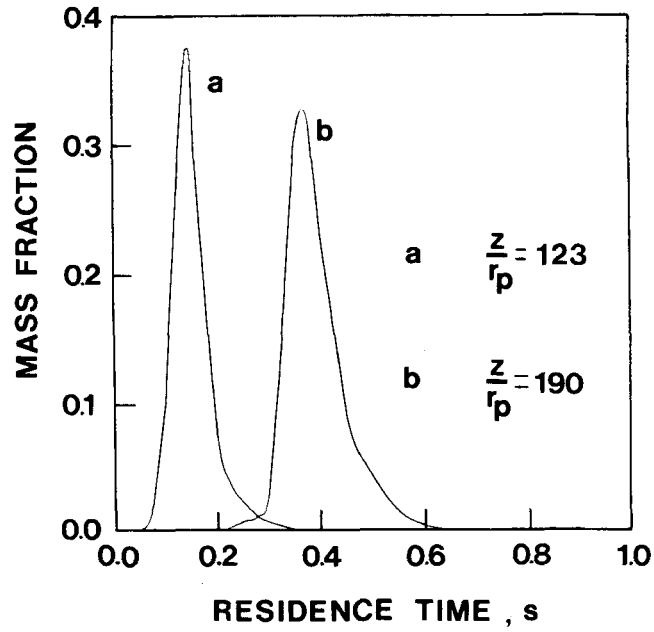

Figure 3. Particle residence time distribution curves.

arising from particle swelling and combustion effects. The incorporation of the coal particle combustion model of Baum and Street (1971) into the model is in progress.

As with any fundamentally based computer simulation, once a solution is determined a large number of parameters of both the gas and solid phases are accessible. Of particular interest here is the particle residence time distribution at various axial locations and Figure 3 shows results for two such locations. These residence time distributions show the expected slightly skewed distribution since the mixing chamber considered in this study can be approximately described as a series of tubular and well-stirred reactors.

NOTATION

a_1, a_2, a_3 = coefficients in Eq. 6
C_D = drag coefficient
C_1, C_2, C_μ = constants in the turbulence model
D_p = particle diameter
k = kinetic energy
Re = $\rho D_p |u_p - u|/\mu$, relative Reynolds number

r_p = radius of primary stream tube (Figures 1–3) instantaneous radial location of particles
t = time
u_p, v_p, w_p = instantaneous components of the particle velocity
u', v', w' = fluctuating components of gas velocity
$\tilde{u}, \tilde{v}, \tilde{w}$ = instantaneous components of the gas velocity
w, r, θ = directions of a cylindrical polar system
z = distance from chamber inlet

Greek Letters

α = defined by Eq. 4
ρ = gas density
ρ_p = particle density
$\mu_{\text{eff}}, \mu, \mu_t$ = effective, laminar and turbulence viscosities
ϵ = rate of dissipation of turbulence energy
ϕ = normally distributed random number
τ = lifetime of a fluid eddy
$\sigma_k, \sigma_\epsilon$ = constants in the turbulence model

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Comments on the Paper, "Gas Transport through Polyethylene Membranes"

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In "Gas Transport through Polyethylene Membranes," [*AIChE J.*, **28**, 474 (1982)] Soles et al. described a procedure for determining both the Henry's Law Constant, H, and the diffusivity, D, which characterize gaseous transport through a polymer membrane. In their experiments, a polymer membrane (either high- or low-density polyethylene) was placed between two reservoirs containing a pure gas initially at different pressures. By assuming one-dimensional diffusion through the membrane, uniform mixing within the reservoirs and equilibrium at the gas-polymer interface, a relationship was derived between D and H and the temporal variation in pressure drop across the membrane. The objectives of their study were threefold:

1) Find a solution to the one-dimensional diffusion equation with the pressure in both reservoirs allowed to vary with time.

2) Find a solution to the one-dimensional diffusion equation for their experimental conditions in which the pressure in one reservoir was essentially constant.

3) Demonstrate a procedure for employing the latter solution to estimate H and D for gaseous transport through a polymer membrane. Soles et al. (1982) determined H and D for the transport of Argon through high- and low-density polyethylene.

Soles et al. (1982) were unable to find a general solution to the problem of one-dimensional diffusion between well-mixed reservoirs and instead reported a solution valid only for short times ($Dt/L^2 \ll 1$). However, solutions for all time are available (Spacek and Kubin, 1967; Shair and Cohen, 1969). The experimental analysis of Soles et al. (1982) was based on the assumption that the pressure in the larger reservoir (the high-pressure reservoir) was essentially constant. While the author's assumption was apparently valid for their experiments, this assumption is not required for analysis of the data. Reible and Shair (1982) employed the solution developed by Shair and Cohen (1969) to determine diffusivities in porous media in an apparatus similar to that employed by Soles et al. (1982). This approach can also be applied to evaluate both H and D in diffusion through polymer membranes and would not be subject to the limitations of the approach by Soles et al. (1982). The objective of the present paper is to outline the application of the solution of Shair and Cohen (1969) to this problem.

PROCEDURE

It is assumed that at time zero a pressure difference is applied across a polymer membrane of length, L, and cross-sectional area, A. The difference in pressure is measured in well-mixed reservoirs of volume V_1 and V_2, on each side of the membrane. At any time, the concentration of the dissolved gas at the edge of the polymer membrane, $C_m(0,t)$ [or $C_m(L,t)$], is in equilibrium with the reservoir pressure, P_1 [or P_2], according to the following relationships

$$P_1(t) = RTC_1(t) = RTHC_m(0,t) \tag{1}$$

$$P_2(t) = RTC_2(t) = RTHC_m(L,t) \tag{2}$$

where H is a Henry's law constant.

In addition, at time zero the dissolved gas concentration throughout the membrane is assumed to be in equilibrium with the pressure