# Calculation of Particle Dispersion Due to Turbulence in Elliptic Flows

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Two-phase combustion such as pulverized coal or droplet spray combustion is commonly encountered in combustion equipment. For realistic predictions, the interaction between the particle phase and the gas phase turbulence must be accurately modeled. As noted by Smoot (1981), the models commonly adopted for modeling particle dispersion are heavily based on empiricism. In these models, the dispersion of particles due to turbulence is assumed to be a diffusional process and is expressed as a gradient of either the mean velocity (Lockwood et al., 1980), or the gradient of the particle bulk number density (Smith et al., 1981). The models, quite clearly, are less than satisfactory, since the basic assumption of relating the dispersion of particles to mean gradients is not well-founded. Further, these models contain empirical constants and there is considerable uncertainty about the suitable values of these constants.

An alternative method has been proposed by Yuu et al. (1978), Dukowicz (1980), and Gosman and Ioannides (1981) in which a stochastic approach to modeling particle dispersion is used. Unlike the empirical approaches, the instantaneous equation for particle motion is solved. Faeth and associates have evaluated this method for parabolic flows (Shuen et al., 1983 a,b; Solomon et al., 1985 a,b,c; Zhang et al., 1985) by comparing the results of the stochastic method with two other two-phase flow models, both of which ignore the turbulent dispersion of particles. However, no comparisons with the empirical models for particle dispersion (Lockwood et al., 1980; Smith et al., 1981) have been made.

The stochastic approach has not been widely used for elliptic flows. We are aware of only four recent studies (Gosman and Ioannides, 1981; Boysan et al., 1986; Boyd and Kent, 1986; Truelove, 1986) where this approach has been used in combustion or furnace geometries. In none of these studies has the performance of the stochastic method been compared with the other models for particle dispersion.

The objective of this paper is to evaluate the performance of the stochastic model for particle dispersion in a turbulent, confined, and recirculating (or elliptic) flow field as encountered in most combustion equipment. Results obtained with the stochastic model will be compared with two other models for turbulent dispersion of particles, those of Lockwood et al. and Smith et al.

#### **Mathematical Models**

In solving for the coupled system of equations for the gas and particles, an Eulerian-Lagrangian formulation described by Crowe et al. (1977) is adopted. Gas-phase equations are solved in an Eulerian framework and models for turbulence, radiation, and combustion must be specified. Turbulence is modeled using the high Reynolds number version of the two-equation  $(k - \epsilon)$  model for turbulence (Launder and Spalding, 1972). The four-flux model for radiation (Gosman and Lockwood, 1974) has been used. For the combustion of volatiles released from the particles (pulverized coal combustion is considered here), a phenomenological model of the "eddy breakup" form proposed by Magnussen and Hjertager (1976) is adopted here.

Particle equations are solved in a Lagrangian framework. The instantaneous and time-averaged equations of particle motion can be respectively expressed as

$$du_{p}/dt = \alpha(u_{e} - u_{p}), dv_{p}/dt = \alpha(v_{e} - v_{p})$$
 (1)

$$d\overline{u}_{p}/dt = \overline{\alpha}(\overline{u}_{g} - \overline{u}_{p}) + \overline{\alpha'(u'_{g} - u'_{p})}, \quad d\overline{v}_{p}/dt$$

$$= \overline{\alpha}(\overline{v}_{g} - \overline{v}_{p}) + \overline{\alpha'(v'_{g} - v'_{p})} \quad (2)$$

where u and v are the axial and radial velocities, and subscripts p and g refer to the particle and gas phases, respectively. The term  $\alpha$  is defined as  $\alpha = 18\mu_g C_D R e_p/24\rho_p^2 d_p$  where  $R e_p$  is the particle Reynolds number and  $C_D$  is the drag coefficient, which is specified according to the expression given by Wallis (1969).

The second term on the righthand side of the time-averaged equations represents the dispersion of the particles due to turbulence in the gas phase, and it is the modeling of this term that is of primary interest in this paper. The three models considered are described in the next section.

For pulverized coal combustion, additional equations must be solved for the particle temperature and combustion of the particle. For purposes of brevity these equations are not given here. The calculation of volatile release from the particle is based on the recommendation of Baum and Street (1971).

# Turbulent dispersion of particles

In this section three models for the turbulent dispersion of particles are described. The first two models solve the time-averaged equation for particle motion and thus require closure for the fluctuating term correlations appearing in these equations. The third model, called the stochastic model, solves the instantaneous equations for particle motion and requires the prescription of the instantaneous gas phase velocities  $u_{\rm g}$  and  $v_{\rm g}$ .

Model 1. Lockwood et al. (1980) have proposed that the effects of turbulent dispersion of particles be incorporated by defining diffusional particle velocities  $\overline{u}_{p,diff}$  and  $\overline{v}_{p,diff}$  due to gas phase turbulence and rewriting Eq. 2 as

$$d\overline{u}_{p}/dt = [18\mu_{g}C_{D}/(24\rho_{p}d_{p}^{2})] \cdot (\overline{\rho}_{g}|\overline{u}_{g} - \overline{u}_{p} - \overline{u}_{p,dif}|d_{p}/\mu_{g})(\overline{u}_{g} - \overline{u}_{p} - \overline{u}_{p,dif})$$
(3)

$$\begin{split} d\overline{v}_{p}/dt &= [18\mu_{g}C_{D}/(24\rho_{p}d_{p}^{2})] \\ &\cdot (\overline{\rho}_{g}|\overline{\overrightarrow{u}}_{g} - \overline{\overrightarrow{u}}_{p} - \overline{\overrightarrow{u}}_{p,dif}|d_{p}/\mu_{g})(\overline{v}_{g} - \overline{v}_{p} - \overline{v}_{p,dif}) \end{split} \tag{4}$$

The diffusional velocities are related to the gas phase turbulence through

$$\overline{u}_{p,diff} = c_1 |\overline{u'^2}| = c_1 |-c_3 2\mu_i/\rho_g(d\overline{u}_g/dx) + \frac{2}{3}k|$$

$$v_{p,diff} = c_2 |\overline{v'^2}| = c_2 |-c_4 2\mu_t/\rho_g(d\overline{v}_g/dy) + \frac{2}{3}k|$$
 (5)

The constants  $c_1$ ,  $c_2$ ,  $c_3$ , and  $c_4$  are specified empirically.

Model 2. In this model (Smith et al., 1981), Eq. 2 is first solved without the turbulent dispersion terms; thus, the computed particle velocities are those that correspond only to the mean gas motion and are denoted by  $\vec{u}_{pc}$  ( $=\vec{i}u_{pc}+\vec{j}v_{pc}$ ). The total particle velocity is obtained by adding a turbulent diffusional velocity  $\vec{u}_{p,diff}$  to  $\vec{u}_{pc}$ , that is,

$$\vec{u}_p = \vec{u}_{pc} + \vec{u}_{p,diff} \tag{6}$$

The diffusional velocity is approximated by a gradient diffusion law:

$$\dot{m}_p^{\prime\prime} = \rho_p^b \overrightarrow{u}_{p,diff} = -\Gamma_p \nabla \rho_p^b = -(\nu_p^l / \sigma_p^l) \nabla \rho_p^b \tag{7}$$

where  $\rho_p^b$  is the bulk particle density,  $\Gamma_p$  is the turbulent particle diffusivity, and  $\nu_p^t$  and  $\sigma_p^t$  are the turbulent particle kinematic viscosity and the turbulent particle Schmidt number, respectively. The relationship proposed by Melville and Bray (1979) is normally used for  $\nu_p^t$ . For  $\sigma_p^t$ , a value of 0.35 has been recommended by Fletcher (1983). The particle bulk density is obtained from the particle number density  $n_p^b$ , which is calculated by solving an Eulerian equation (Fletcher, 1980). This model is the most commonly adopted approach for incorporating the effects of turbu-

lence on particle dispersion (Fletcher, 1980, 1983; Smith et al., 1981).

Stochastic Model. In the stochastic model (Gosman and Ioannides, 1981; Shuen et al., 1983a,b), Eq. 1 is solved directly in its instantaneous form. The particle is assumed to interact with a succession of eddies as it traverses the flow. The properties in each eddy are assumed to be uniform but change randomly from one eddy to the next. Since Eq. 1 is solved in its instantaneous form, instantaneous eddy properties are required. These are obtained by assuming isotropic turbulence and making a stochastic selection from the Gaussian velocity probability distribution function with mean  $\overline{u}_g$  and variance 2k/3. Both  $\overline{u}_g$  and k are obtained from the gas phase calculations.

The particle is assumed to interact with the eddy if its displacement within the eddy is smaller than a characteristic eddy size  $\ell_e$ , and the time of interaction is smaller than the characteristic eddy life time  $t_e$ . Conventional expressions for the eddy size and lifetime are (Gosman and Ioannides, 1981),

$$\ell_e = c_\mu^{3/4} k^{3/2} / \epsilon, \, t_e = \ell_e / (2k/3)^{1/2} \tag{8}$$

An important consideration is that of specifying the correct instantaneous particle conditions at the inlet. The importance of the inlet particle fluctuation terms can be noted from the reported measurements of Shuen et al. (1983b) in a particle-laden jet. Since, in general, inlet particle fluctuation measurements are not reported, an alternative approach to predicting these terms has to be devised.

In this paper a relatively simple approach has been developed to predict the particle fluctuation terms at the inlet of the furnace. The calculation domain is extended upstream of the inlet to include a certain length of inlet pipe carrying the particle-air mixture. Since the cross-stream particle fluctuations dictate the particle dispersion in the radial direction, calculations for the instantaneous cross-stream velocities in the inlet pipe are done by the stochastic method outlined above. Fully developed turbulent gas flow is assumed in the pipe with zero mean cross-stream velocities, and  $\overline{u}_p = \overline{u}_g$ . Eddy size information is obtained from the experimental data for mixing length (Davies, 1972). To calculate instantaneous eddy properties, a Gaussian probability distribution function is assumed with the mean value obtained from the assumption of fully developed pipe flow and the variance from the assumption of 10% turbulent intensity in the pipe. At the entrance to the pipe, for each particle size group, a massweighted radial location is calculated assuming uniform radial distribution of particles. Stochastic calculations for this particle size group are initiated from its mass-weighted location and continued to the end of the inlet pipe, which coincides with the inlet to the furnace. By this procedure, the particle velocities at the end of the inlet pipe are computed for each particle size group and are used to characterize the inlet particle condition at each radial location at the combustor inlet.

## **Results and Discussion**

Three sets of measurements have been chosen to make performance evaluations. The first two sets (Memmott, 1977; Leavitt, 1980) correspond to isothermal, two-phase flow in a cylindrical combustor geometry. Particles in the range of 5-160  $\mu$ m were used in these experiments. The third set of data was obtained by Michel and Payne (1980) for pulverized coal flame (15-250  $\mu$ m

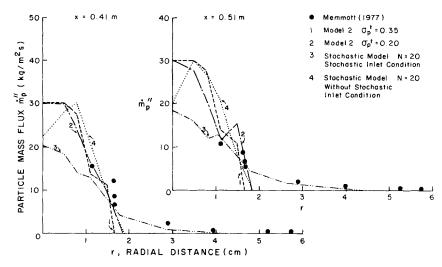


Figure 1. Model evaluation, isothermal flow data of Memmott (1977).

particles) in a rectangular geometry which, in this study, has been replaced by a cylindrical geometry with the same equivalent diameter.

It should be noted that in the configurations considered, the near field of the inlet is characterized by strong adverse and radial pressure gradients, and radial velocities. Thus the injected particles clearly experience the flow field ellipticity.

# Sensitivity tests

The sensitivity of the stochastic method to the number of stochastic calculations for each particle size group and starting location is an important factor in controlling the overall computational cost. This consideration is particularly important for the computer-intensive calculation of elliptic flows. Therefore, a sensitivity test is performed, and results are obtained with 5, 20, 40, 100, and 200 stochastic calculations for each particle size group and starting location and compared with the isothermal data of Memmott (1977).

It is observed that the predictions with 20, 40, 100, and 200 stochastic calculations per particle size group and starting location agree well with each other and also with the measured values. With five stochastic calculations per particle size group and starting location, local discrepancies are noted. Therefore, it

appears that 20 stochastic calculations per representative particle trajectory are sufficient for elliptic, isothermal flows. This observation is also verified for reacting flows, as shown by Figure 3.

#### Model Evaluation

In this section the predictions for particle dispersion using models 1 and 2 and the stochastic model are compared with one another.

Isothermal Flow. Since model 2 has been the most popular approach heretofore, isothermal flow predictions have been obtained using model 2 and the stochastic method. In view of the uncertainty associated with the value of  $\sigma_p^t$  in model 2, predictions have been obtained using the recommended value of 0.35 (Fletcher, 1983) and 0.2.

Figure 1 shows the comparison between the predictions and the data of Memmott (1977) at two axial locations. Predictions using model 2 exhibit a steep radial decay in particle flux, with near-zero values beyond r = 2.0 cm. However, the measurements indicate a greater level of the radial dispersion of particles, with the particle flux gradually decaying to zero at r = 4.0 cm. Predictions using the stochastic method exhibit these measured trends and, quite clearly, provide more realistic simula-

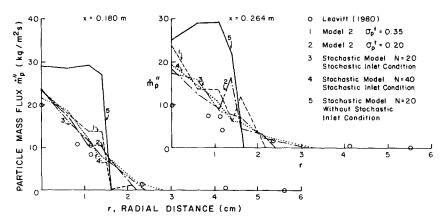


Figure 2. Model evaluation, isothermal flow data of Leavitt (1980).

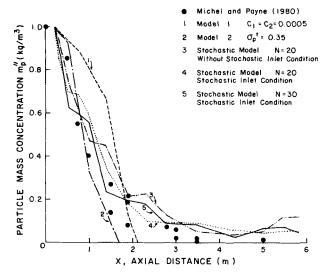


Figure 3. Model evaluation, reacting flow data of Michel and Payne (1980).

tions than those obtained using model 2. Both choices of  $\sigma_p^t$  yield nearly similar radial profiles, with somewhat greater radial dispersion predicted at the lower  $\sigma_p^t$  value.

The effect of specifying the particle velocity fluctuations at the inlet, using the simple stochastic approach described earlier, is shown in Figures 1 and 2. Quite clearly, the effects are significant, and for realistic predictions with the stochastic method, the inlet particle velocity fluctuations must be included.

The validity of the simple stochastic method used for predicting the inlet particle velocity fluctuations may also be noted by comparing  $(\sqrt{v_p'^2}/\overline{u}_p)_{inlet}$  predicted in this study with the measurements in Shuen et al. (1983b). The two values agree well with each other. Although the two flow conditions in the two inlet pipes are somewhat different, the same order of magnitude of the two values indicates the validity of the approach.

Figure 2 shows the comparison of predictions with the data of Leavitt (1980), and observed trends are consistent with those in Figure 1. Model 2 profiles exhibit rather nonuniform behavior. These nonuniformities can be reduced by increasing the number of particle starting locations and particle size groups, but the radial dispersion of particles is always underpredicted when model 2 is used.

Reacting Flow. Pulverized coal combustion predictions using model 1, model 2, and the stochastic method are compared with the data of Michel and Payne (1980) in Figure 3. Model 1 predictions compare rather poorly with the measured values, while the solutions obtained using model 2 do not agree with the measurements beyond X=2.0 m.

Predictions with the stochastic method appear to agree well with the measured values. The axial distribution without inlet particle velocity fluctuations exhibit satisfactory agreement with the data, but the radial distributions (not shown) indicate local differences between predictions and measurements, and again point to the importance of incorporating particle velocity fluctuations at the inlet.

Figure 3 also shows the effect of increasing the number of stochastic calculations per size group and starting location from 20 to 30. The predicted profiles, as in isothermal flows, show close agreement to each other.

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## **Notation**

 $c_1, c_2, c_3, c_4, c_\mu = \text{empirical constants}; c_1 = c_2 = 0.0005; c_3 = c_4 = 1; c_\mu = 0.0005; c_3 = 0.0005; c_4 = 0.0005; c_5 = 0.0005; c_6 = 0.0005; c_8 = 0.0005;$ 0.09 $c_D = \text{dimensionless drag coefficient}$  $d_p$  = particle diameter, m  $\dot{k}$  = turbulent kinetic energy per unit mass, J/kg l, = eddy size  $i' = particle mass flux, kg/m^2 \cdot s$ = particle mass concentration, kg/m<sup>3</sup> N = number of stochastic calculations per particle size group and starting location = bulk particle number density, m<sup>-3</sup> r = radial distance from the centerline, cm or m  $Re_p = \text{particle Reynolds number}$ t = time, su, v, u', v' = velocity and fluctuating velocity components, m/s X =axial distance from burner exit, m or cm

#### Greek letters

 $\alpha$  = coefficient in particle trajectory equation  $\Gamma_{\rho}$  = turbulent particle diffusivity =  $\nu'_{\rho}/\sigma'_{\rho}$ ,  $m^2/s$   $\epsilon$  = turbulence energy dissipation rate,  $J/kg \cdot s$   $\mu$  = dynamic viscosity, kg/ms  $\nu'_{\rho}$  = turbulent particle kinematic viscosity,  $m^2/s$   $\rho^2_{\rho}$  = bulk particle mass density,  $kg/m^3$   $\sigma^2_{\rho}$  = turbulent particle Schmidt number

### Literature Cited

Baum, M. M., and P. J. Street, "Predicting the Combustion Behavior of Coal Particles," *Combust. Sci. Tech.*, 3, 231 (1971).

Boyd, R. K., and J. H. Kent, "Three-Dimensional Furnace Computer Modeling," 21st Symp. (Int.) on Combustion, Munich (Aug., 1986).

Royson, F. R. Weber, I. Swithenbank, and C. I. Lawn, "Modeling

Boysan, F., R. Weber, J. Swithenbank, and C. J. Lawn, "Modeling Coal-Fired Cyclone Combustors," Combust. Flame, 63, 73 (1986).

Crowe, C. T., M. P. Sharma, and D. E. Stock, "The Particle Source in Cell (PSI-Cell) Model for Gas-Droplet Flows," J. Fluids Eng., 99, 325 (1977).

Davies, J. T., Turbulence Phenomena, Academic Press, 19 (1972).

Dukowicz, J. K., "A Particle-Fluid Numerical Model for Liquid Sprays," J. Comp. Phys., 35, 229 (1980).

Fletcher, T. H., "Theoretical Modeling of Reacting Coal Particles in Pulverized Coal Combustion and Gasification," M.S. Thesis, Dept. Chem. Eng., Brigham Young Univ., Provo, UT (1980).

-----, "A Two-Dimensional Model for Coal Gasification and Combustion," Ph.D. Diss., Dept. Chem. Eng., Brigham Young Univ., Provo, UT (1983).

Gosman, A. D., and E. Ioannides, "Aspects of Computer Simulation of Liquid-Fueled Combustors," AIAA Paper No. 81-0323 (1981).

Gosman, A. D., and F. C. Lockwood, "Incorporation of a Flux Model for Radiation into a Finite-Difference Procedure for Surface Calculations," 14th Symp. (Int.) on Combustion, Combustion Inst., Pittsburgh (1974).

Launder, B. E., and D. B. Spalding, Mathematical Models of Turbulence, Academic Press, London (1972).

Leavitt, D. R., "Coal Dust and Swirl Effects on Gas and Particle Mixing Rates in Confined Jets," M.S. Thesis, Dept. Chem. Eng., Brigham Young Univ., Provo, UT (1980).

Lockwood, F. C., A. P. Salooja, and S. A. Syed, "A Prediction Method for Coal-Fired Furnaces," Combust. Flame, 38, 1 (1980).

Magnussen, B. F., and H. Hjertager, "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion," 16th Symp. (Int.) on Combustion, Combustion Inst., Pittsburgh, 719 (1976).

Melville, E. K., and K. N. C. Bray, "A Model of the Two-Phase Turbulent Jet," Int. J. Heat Mass Trans., 22, 647 (1979).

Memmott, V. J.,. "Rates of Mixing of Particles and Gases in Confined

- Jet," M.S. Thesis, Dept. Chem. Eng., Brigham Young Univ., Provo, UT (1977).
- Michel, J. B., and R. Payne, "Detailed Measurements of Long Pulverized Coal Flames for the Characterization of Pollutant Formation," IFRF Doc. No. F09/a/23, Ijmuiden, The Netherlands (1980).
- Shuen, J. S., L. D. Chen, and G. M. Faeth, "Evaluation of a Stochastic Model of Particle Dispersion in a Turbulent Round Jet," AIChE J., 29, 167 (1983a).
- , "Predictions of the Structure of Turbulent Particle-Laden Round Jets," AIAA J., 21, 1483 (1983b).
- Smith, P. J., T. J. Fletcher, and L. D. Smoot, "Model for Pulverized Coal-Fired Reactors," 18th Symp. (Int.) on Combustion, Combustion Inst., Pittsburgh, 1285 (1981).
- Smoot, L. D., "Pulverized Coal Diffusion Flames—A Perspective Through Modeling," 18th Symp. (Int.) on Combustion, Combustion Inst., Pittsburgh, 1185 (1981).
- Solomon, A. S. P., J. S. Shuen, Q. F. Zhang, and G. M. Faeth, "Structure of Nonevaporating Sprays. I: Near-Injector Conditions and Mean Properties," AIAA J., 23, 1548 (1985a).

- ----, "Structure of Nonevaporating Sprays. II: Drop and Turbulent Properties," AIAA J., 23, 1724 (1985b).
- , "Measurements and Predictions of the Structure of Evaporating Sprays," J. Heat Trans., 107, 679 (1985c).

  Truelove, J. S., "Prediction of the Near-burner Flow and Combustion
- Truelove, J. S., "Prediction of the Near-burner Flow and Combustion in Swirling Pulverized Coal Flames," 21st Symp. (Int.) on Combustion, Munich (Aug., 1986).
- Wallis, G. B., One-Dimensional and Two-Phase Flow, McGraw-Hill, New York (1969).
- Yuu, S., N. Yasukouchi, Y. Hirosawa, and I. Jotaki, "Particle Turbulent Diffusion in a Dust-Laden Round Flame," AIChE J., 24, 509 (1978).
- Zhang, Q. F., J. S. Shuen, A. S. P. Solomon, and G. M. Faeth, "Structure of Ducted Particle-Laden Jets," AIAA J., 23, 1123 (1985).

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