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Technical Notes

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Probability Density Function Shape Sensitivity in the Statistical Modeling of Turbulent Particle Dispersion

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Introduction

A STATISTICAL transport model for turbulent particle dispersion having significant potential for improving the efficiency and robustness of computational fluid dynamics (CFD) analyses for particle laden flows was recently introduced in this journal.[1] The technique described as a stochastic-dispersion-width-transport (SDWT) model was based on coupling a stochastic direct-modeling approach for parcel/eddy interaction properties with continuous probability density functions (pdf) to describe the physical particle temporal and spatial distribution. More specifically, a computational parcel representing a group of physical particles is characterized by a normal pdf in space. The mean of each pdf is determined by Lagrangian tracking of a computational parcel through a sequence of stochastically generated turbulent eddies. The variance of each pdf is represented by a turbulence-induced mean square dispersion as determined from a statistical formulation based on the linearized particle equations of motion. This technique provides reduced sampling requirements with minimal induced numerical noise and was shown to produce good time-averaged dispersion results in comparison with the conventional direct-modeling approach. A Technical Note addressing additional computational efficiency has also been presented in this journal[2] in which a truncation criterion was developed for limiting the perturbing influence of a turbulent eddy to subsequent interactions in which it makes a nonnegligible contribution. This truncation was introduced to eliminate unnecessary and redundant computations.

In all of the previous work, however, the parcel pdf shape was assumed normal (Gaussian). In seeking greater efficiency and simplicity for practical implementation, it is of interest to investigate the sensitivity of the model to alternative pdf shapes. In this Note, the performance of the model using both uniform and isosceles triangle pdfs is studied for rigid particles injected into a round turbulent jet.

Theory

From a theoretical standpoint, the normal pdf characterization of a parcel approaches an exact representation of the actual diffusive-type particle dispersion observed in certain turbulent flows. This was demonstrated by the SDWT model for nearly homogeneous turbulent flow and a round turbulent jet in a previous publication.[1] In the SDWT model, the normal distribution function may also be deduced as a result of the Central Limit Theorem from probability theory that states that the sum of a large number of mutually independent, identically distributed random variables is approximately normal. Theoretically, therefore, a normal pdf is the best parcel characterization. But from a practical standpoint, simplicity in computing the distribution of physical particles over a computational grid is important in terms of efficiency, and relaxation of the normal pdf parcel representation to simpler alternative pdf shapes may be desirable. It is difficult to quantify the potential gains in efficiency one might obtain using such alternative pdf shapes since it would ultimately depend on problem geometry and coding technique, but the potential for improvement certainly exists. Between the extremes of a delta-function pdf as used in the conventional stochastic-separated-flow (SSF) technique and the theoretically optimal normal pdf, we seek to examine SDWT model sensitivity to both uniform and isosceles triangle pdf parcel characterizations.

In the most general three-dimensional case, integration over three spatial coordinates is required to determine the probability of locating a physical particle at a given position. This evaluation may be made simpler for an axisymmetric flow such as a round turbulent jet where turbulent dispersion effects in the axial direction are relatively weak with respect to that of transverse dispersion. This was the test case used for initial evaluation of the SDWT model with a normal pdf parcel characterization, and it will be re-examined here for pdf shape sensitivity. By neglecting the mild dispersive effect in the flow direction, integration over the parcel pdf is required only in planes transverse to the flow. Statistically, we impose the constraint of a negligible standard deviation $\sigma_{ax} \rightarrow 0$ for the axial coordinate.

The integration is performed by considering a single-coordinate pdf in a plane parallel to and intersecting the axis of symmetry with a mean r_p and a standard deviation σ_r as shown in Fig. 1 for a uniform and an isosceles triangle pdf. These pdfs are defined as follows, where evaluation of the second moment about the mean gives a relation between the standard deviation σ_r and the half-width w:

Uniform pdf:

$$f(r) = \begin{cases} 0, & r \leq r_p - w \\ \dfrac{1}{2w}, & r_p - w < r < r_p + w \\ 0, & r \geq r_p + w \end{cases} \tag{1}$$

$$w = \sqrt{3}\sigma_r \tag{2}$$

Isosceles triangle pdf:

$$f(r) = \begin{cases} 0, & r \leq r_p - w \\ \dfrac{1}{w^2}(r - r_p + w), & r_p - w < r \leq r_p \\ \dfrac{-1}{w^2}(r - r_p - w), & r_p < r < r_p + w \\ 0, & r \geq r_p + w \end{cases} \tag{3}$$

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$$w = 2\sqrt{3}\sigma_r \tag{4}$$

Then an axisymmetric cumulative distribution function at any radius r may be defined as the volume swept out by the planar region of the pdf bounded by $-r \leq R \leq r$ as it is revolved 360 deg about the axis of symmetry. For these pdfs, there are two fundamental cases to consider, depending on whether the symmetry axis intersects the distribution or not. After integration, the resulting cumulative distribution function $F(r)$ is normalized by $F(r \rightarrow \infty)$ to obtain the axisymmetric probability of locating a physical particle within a given radius r. The following forms were obtained:

Uniform pdf:

Case 1: $r_p < w$

$$P(r) = \frac{F(r)}{F(r \rightarrow \infty)} = \begin{cases} \dfrac{r^2}{r_p^2 + w^2}, & r \leq w - r_p \\ \dfrac{r^2 + (w - r_p)^2}{2(r_p^2 + w^2)}, & w - r_p < r < w + r_p \\ 1, & r \geq w + r_p \end{cases} \tag{5}$$

Case 2: $r_p \geq w$

$$P(r) = \frac{F(r)}{F(r \rightarrow \infty)} = \begin{cases} 0, & r \leq r_p - w \\ \dfrac{r^2 + (r_p - w)^2}{4 r_p w}, & r_p - w < r < r_p + w \\ 1, & r \geq r_p + w \end{cases} \tag{6}$$

Isosceles triangle pdf:

Case 1: $r_p < w$

$$P(r) = \frac{F(r)}{F(r \rightarrow \infty)} = \begin{cases} \left\{ \begin{array}{ll} \dfrac{6(w - r_p)r^2}{-2r_p^3 + (w + r_p)^3 + (w - r_p)^3}, & r \leq r_p \\ \dfrac{-4r^3 + 6wr^2 - 2r_p^3}{-2r_p^3 + (w + r_p)^3 + (w - r_p)^3}, & r > r_p \end{array} \right\} & r \leq w - r_p \\ \left\{ \begin{array}{ll} \dfrac{2r^3 + 3(w - r_p)r^2 + (w - r_p)^3}{-2r_p^3 + (w + r_p)^3 + (w - r_p)^3}, & r \leq r_p \\ \dfrac{-2r^3 + 3(w + r_p)r^2 - 2r_p^3 + (w - r_p)^3}{-2r_p^3 + (w + r_p)^3 + (w - r_p)^3}, & r > r_p \end{array} \right\} & w - r_p < r < w + r_p \\ 1, & r \geq w + r_p \end{cases} \tag{7}$$

Case 2: $r_p \geq w$

$$P(r) = \frac{F(r)}{F(r \rightarrow \infty)} = \begin{cases} 0, & r \leq r_p - w \\ \left\{ \begin{array}{ll} \dfrac{2r^3 - 3(r_p - w)r^2 + (r_p - w)^3}{-2r_p^3 + (r_p + w)^3 + (r_p - w)^3}, & r \leq r_p \\ \dfrac{-2r^3 + 3(r_p + w)r^2 - 2r_p^3 + (r_p - w)^3}{-2r_p^3 + (r_p + w)^3 + (r_p - w)^3}, & r > r_p \end{array} \right\} & r_p - w < r < r_p + w \\ 1, & r \geq r_p + w \end{cases} \tag{8}$$

Results

Statistical sensitivity to the parcel pdf shape is demonstrated for time-averaged dispersion of rigid, nonevaporating particles injected into a round turbulent jet. Based on the SDWT theoretical development, an ensemble of particles represents a group of pdfs that, upon convolution, yield the probable physical particle distribution. By performing the convolution with alternate pdf shapes, model sensitivity is examined.

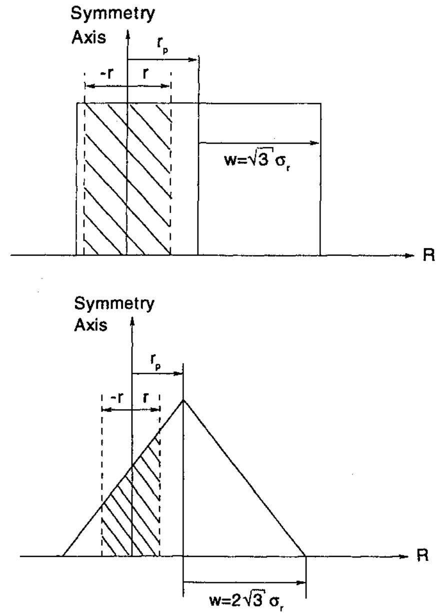

Fig. 1 Parcel pdf in a plane parallel to and intersecting the axis of symmetry; a) uniform pdf, b) isosceles triangle pdf.

The round turbulent air jet used in the initial model evaluation study[1] is re-examined in the current study. To recapitulate, the jet is directed upward against gravitational acceleration from a nozzle 2.18 cm in diameter with a mean exit velocity of 26 m/s. For demonstration purposes, particles with a diameter of 50 μm and a density of 1000 kg/m^3 are ejected at the mean nozzle exit velocity. Under the dilute spray as-

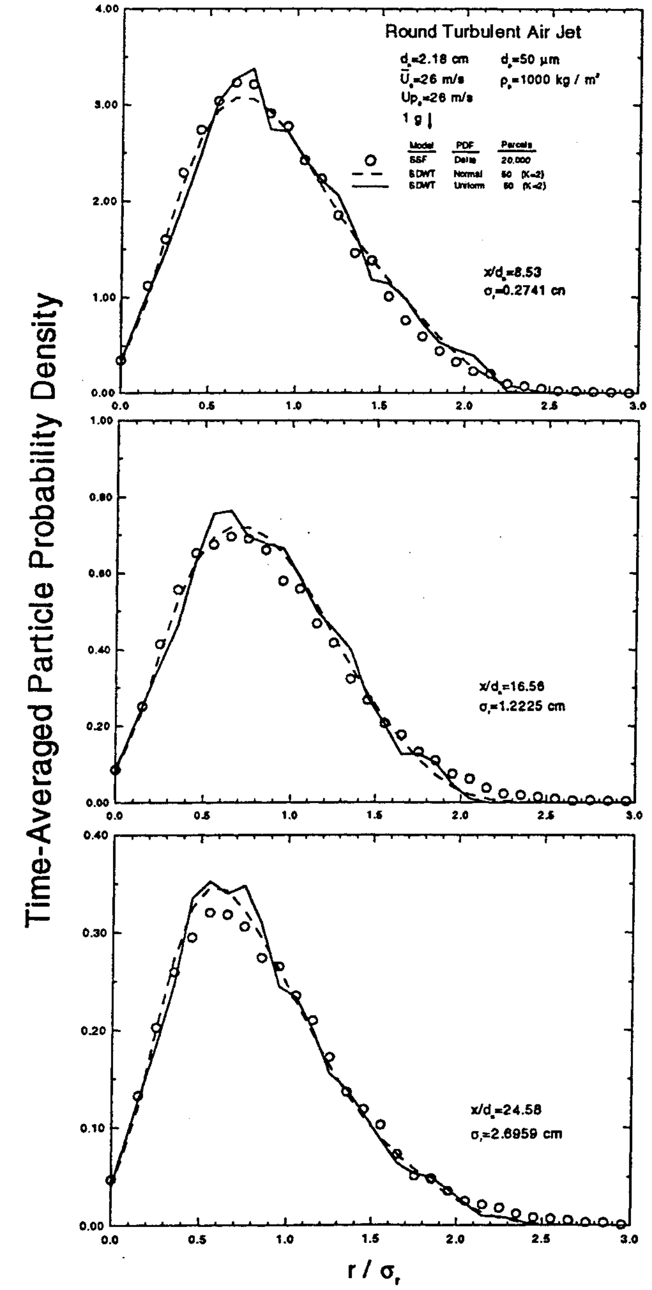

Fig. 2 Predicted time-averaged physical particle pdf using uniform parcel pdfs.

sumption, particle loading on the gas phase was neglected. The jet was divided into 30 radial cells at each cross section of interest.

For a comparative baseline, the time-averaged physical particle pdf was first obtained from the SSF model formulation with delta-function parcel characterization using a 20,000 particle sample and from SDWT theory using normal pdfs on a 50-parcel ensemble with an undersampling correction factor of $K = 2$. The 50-parcel ensemble provided sufficient sampling for obtaining a smooth, accurate distribution for the baseline case. The time-averaged dispersion was then recomputed from SDWT theory using both uniform and triangular pdfs on the 50-parcel ensemble. In these calculations, $K = 2$ for the uniform pdf and $K = 1.5$ for the triangular pdf. The principal effect and purpose of K is to amplify the magnitude of the dispersion width, but because the half-width of the triangular pdf is quite large, a reduced value of K proves satisfactory. Results for the preceding calculations are shown in Figs. 2 and 3, respectively.

When using a uniform parcel pdf, the resulting distribution is found to trace through the baseline predictions, but it is also observed to be highly irregular. Such irregularity implies that interphase transport source effects will fluctuate in space and time, resulting in computational shot noise. Although not overly important in many engineering calculations, this numerically induced noise can be unacceptable in unsteady analyses aimed at assessing flow stability. The source of the irregularity in the predicted physical particle distribution stems from the absence of tails in the uniform pdf. On the other hand, because the triangular pdf better approximates the tails of the normal pdf, its predicted physical particle distribution is found to perform exceptionally well. In this case, the resulting distribution exhibits no irregular features and is almost indistinguishable from the baseline results. The distribution exhibits a high degree of smoothness, indicating minimal potential for inducing numerical noise.

For implementing SDWT theory into a practical computational analysis, it may be advantageous to apply an isosceles triangle pdf parcel characterization. The resulting algorithmic

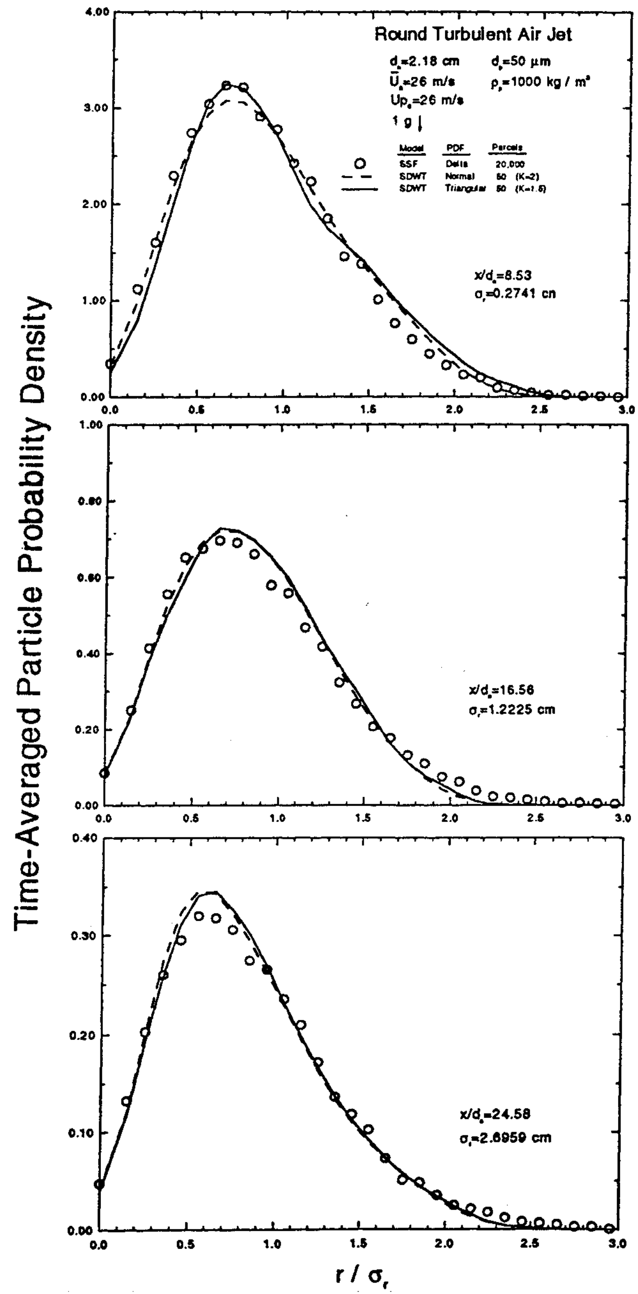

Fig. 3 Predicted time-averaged physical particle pdf using isosceles triangle parcel pdfs.

simplification in calculating the physical particle distribution over a grid could mean substantial gains in code efficiency. Moreover, there will be virtually no accompanying increase in numerical noise generation as compared with predictions using normal pdfs. In some cases, it may also be acceptable to apply the theory with the even simpler uniform pdfs where rapid computation of an approximate solution is desired.

Acknowledgments

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Statistical Modeling of Turbulent Dilute Combusting Sprays

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Introduction

THIS Note comments on the application of a new statistical transport model for turbulent particle dispersion[1-3] to dilute combusting sprays. The approach taken was to examine model performance with respect to available experimental data. Comparison with predictions using a conventional direct modeling technique was also made. The particular test conditions for the experiment may be described as a dilute monodispersed spray of fuel droplets injected into a round, turbulent diffusion flame. Our primary interest in this work was to justify the use of the statistical transport model for combusting droplets and to demonstrate the potential for improved efficiency with minimal sacrifice in accuracy.

Approach

The fundamental data reported by Shuen et al.[4,5] proved very useful because of the simple test configuration of their experiments. The flow conditions produced may be well characterized by established theoretical methods allowing computation of the detailed flowfield. The physical conditions of their experiments are fully described in Ref. 5. Here we provide a brief summary of the test arrangement. Methane is vertically injected upward through a converging nozzle with a throat diameter of 5 mm. The exit Reynolds number is 1.17×10^4 with a centerline velocity of 52.8 m/s. The injection temperature is a nominal 300 K. The resulting fully turbulent diffusion flame burns in stagnant air at atmospheric pressure. A dilute monodisperse spray of methanol droplets was introduced with initial drop diameters of 105 and 180 μm. The spray injection rates are summarized in Table 1.

To evaluate the proposed dispersion model, numerical methods are used to compute the mean background flow for the turbulent diffusion flame. With the proper initial/boundary conditions known from measurements, the continuous-phase analysis may be performed and validated against flame structure data. The calibrated theoretical solution then provides the necessary flowfield resolution to evaluate dispersion models.

The theoretical methods of Jeng and Faeth[6] are employed for the continuous-phase analysis. For the dilute spray assumption, drop source terms in the continuous phase are ignored. Furthermore, boundary-layer approximations are applicable so that the governing flow equations become parabolic. Jeng and Faeth's method for analyzing this flow involves solution of a Favre-averaged formulation due to Bilger[7] with a κ-ϵ-g turbulence closure. By introducing a conserved-scalar (mixture fraction) formalism, the governing equations are solved for mean conservation of mass, momentum, and mixture fraction. Instantaneous scalar properties are then determined from the mixture fraction probability density functions (pdf) with appropriate state relationships.

Applying a two-parameter clipped Gaussian function for the Favre pdf, the mean and variance are computed from the known mixture fraction and square mixture fraction fluctuation as described by Lockwood and Naguib.[8] With the Favre pdf fully defined, Favre-averaged values of all scalar properties may then be computed. A relation also exists for obtaining time-averaged mean quantities. The necessary state relationships are constructed according to the laminar flamelet method of Bilger[9] and Liew et al.[10] This method is based on the observation that temperature and species concentrations in laminar diffusion flames are nearly unique functions of mixture fraction alone. Laminar flamelet correlations are then developed from laminar flame measurements and applied to turbulent diffusion flames. This is accomplished by viewing a turbulent flame as a sequence of laminar flamelets passing a given location in the flow. Jeng and Faeth[6] constructed the state relationship for methane burning with air from laminar flame measurements.

Our statistical treatment of turbulent sprays may be described as a stochastic-dispersion-width-transport (SDWT) model. It is based on coupling a direct modeling approach for particle/eddy interactions with continuous two-parameter probability density functions to describe the physical particle spatial and temporal distribution. In the current formulation, a computational parcel is represented by a normal pdf in space. The mean of each pdf is determined by Lagrangian tracking of each parcel through a sequence of stochastically generated turbulent eddies. The variance of each pdf is represented by a turbulence-induced mean square dispersion as determined from a statistical formulation based on the linearized particle equations of motion. Convolution of the parcel pdfs yields the probable physical particle distribution at a given instant in time. Full details of the theoretical formulation are available in previous publications.[1-3]

Like Shuen et al.,[4,5] we also examine the basic stochastic-separated-flow (SSF) direct modeling approach, which is recovered as a special case of the SDWT model by introducing a delta-function representation for each computational parcel.

Table 1 Spray injection rates

Nominal drop diameter, μm	105	180
Liquid volume flow rate, μl/s	12.21	24.48
Nominal injection rate, drops/s	20,000	8,000

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