# Efficient Statistical Transport Model for Turbulent Particle Dispersion in Sprays

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**A statistical transport model for turbulent particle dispersion is formulated having significantly improved computational efficiency in comparison to the conventional stochastic discrete-particle methodology. In the proposed model, a computational parcel representing a group of physical particles is characterized by a normal (Gaussian) probability density function (pdf) in space. The mean of each pdf is determined by Lagrangian tracking of each computational parcel, either deterministically or stochastically. The variance of each pdf is represented by a statistically derived turbulence-induced mean square dispersion from the linearized direct modeling formulation for particle–eddy interactions. Convolution of the computational parcel pdfs produces the probable distribution of particles in the spray. The validity of the new model is established for time-averaged dispersion by comparison with the conventional stochastic direct modeling method, wherein each parcel is represented by a discrete delta function in space, for nonevaporating particles injected into simple turbulent air flows.**

## Nomenclature

$A$ = defined variable, Eq. (14)
$C_\mu$ = turbulence model constant, 0.09
$C_D$ = drag coefficient, $= 24(1 + Re^{2/3}/6)/Re$ ; $Re < 1000$
$= 0.44$ ; $Re \geq 1000$
$d$ = diameter, m
$F$ = cumulative distribution function
$g$ = gravity, 9.81 m/s$^2$
$K$ = undersampling correction factor
$k$ = turbulent kinetic energy, m$^2$/s$^2$
$L_e$ = eddy dissipation length scale, m
$N_{cp}$ = number of computational parcels
$N_{pp}$ = number of physical parcels
$P$ = probability
$r$ = radial coordinate, m
$t$ = time, s
$T_k$ = dispersion transport factor from $k$th eddy to $n$th eddy
$u$ = velocity, m/s
$x$ = displacement, m
$z, Z$ = dummy variables
$\Delta$ = relative change
$\varepsilon$ = turbulent energy dissipation rate, m$^2$/s$^3$
$\rho$ = density, kg/m$^3$
$\sigma$ = standard deviation of pdf, m
$\sigma^2$ = variance of pdf or mean squared dispersion, m$^2$
$\tau$ = particle relaxation time,
$(4/3)(\rho_p/\rho_g)(d_p/C_D)(1/|u_g - u_p|)$, s
$\Phi$ = standardized normal cumulative distribution function

*Subscripts and Superscripts*

$ax$ = axial coordinate
$e$ = eddy
$(e)$ = computational parcel ensemble
$g$ = gas phase, gravity
$int$ = interaction quantity
$i$ = interaction index
$j$ = interaction index
$k$ = interaction index
$l$ = interaction index
$n$ = interaction index, nozzle
$p$ = particle or parcel
$r$ = radial coordinate
$rms$ = root mean square
$t$ = transit of eddy by particle
$'$ = turbulence quantity
$0$ = initial condition
$\bar{}$ = mean value
$\hat{}$ = normalized quantity

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## Introduction

COMPUTATIONAL fluid dynamics analysis of turbulent, two-phase, reacting flows finds useful applications in the design and development of many power production devices involving spray combustion. The immense costs and time requirements associated with experimental trial-and-error development methods, as well as the extensive insight derivable from a detailed analysis, warrant the establishment of ever more comprehensive predictive capabilities. Modeling the complex physical phenomena of turbulence, chemical reaction, and interphase transport, however, can introduce such excessive computational requirements that numerical simulation becomes impractical. Therefore, maintaining computational efficiency is crucial in the pursuit of ever more sophisticated analyses.

The general philosophy of spray combustion modeling has been greatly influenced by these computational constraints. For example, the massive number of particles typically encountered in practical systems generally make a statistical description of group behavior necessary—therein the introduction of continuous statistical distribution functions and the discretization concept whereby a continuous distribution function is replaced by discrete delta functions (that is, groups of physical particles are represented by single parcels each characterized by a single point in space). The collective behavior of particle interactions with the continuous gas phase is, thus, a major focus of spray modeling efforts.

Primarily, spray combustion models have been classified as either locally homogeneous-flow (LHF) models, where the condensed phase is assumed to be in local dynamic and thermodynamic equilibrium with the gas phase, or separated-flow

(SF) models, where finite-rate interphase transport is considered.[1,2] The results of various studies have indicated that LHF models overestimate the rate of development of the process and are basically unsuitable for most spray combustion flows. SF models, considering finite-rate interphase exchange of mass, momentum, and energy have been more desirable, therefore, because of their more comprehensive nature.

A common SF approach is the discrete-particle model (DPM), as exemplified by the method of Crowe et al.,[3] in which the physical spray is represented by a finite number of computational parcels. From a statistical point of view, each computational parcel is characterized by a delta function in space which is treated as a single effective particle for tracking but otherwise represents a group of real physical particles for the purpose of evaluating interphase transport. Indeed, the computational parcels are tracked using a Lagrangian formulation, a distinct advantage since numerical diffusion is minimized. Furthermore, their life histories are determined from discrete particle gasification models. Source terms are also introduced into the Eularian gas-phase conservation equations according to the distribution of parcels. The central disadvantage of a DPM is the point source representation for groups of physical particles which can introduce computational shot noise when an insufficient number of computational parcels are used such that large fluctuating transport sources are generated in space and time.

An alternative SF approach is the continuous-particle model (CPM) as proposed by Williams.[4] In this approach, a multidimensional statistical distribution function, avoiding the point source restriction, gives a field description of particle properties. The distribution function is treated as a continuous property of the flow, and a phenomenologically derived Eularian transport equation for this function is solved with the gas-phase equations containing appropriate source terms. The main difficulties with CPM are the multidimensions of the distribution function when considering a multiplicity of particle properties and the strong spatial gradients associated with these properties which require very fine grid spacing to reduce numerical diffusion.[1,2] The resulting computer storage requirements and increase in computational time can be prohibitive.

A third SF method for modeling sprays is the continuum-formulation model (CFM), in which the gas and dispersed phase are treated as an interpenetrating continua. This formulation results in similar governing equations for both phases, which can become dubious when attempting to represent turbulent stresses and interphase transport. Since multiple fluid phases must be considered for various ranges in particle size, CFM becomes costly in terms of computational time and storage requirements.[1,2]

Of the three SF spray combustion model categories (DPM, CPM, CFM), DPMs are the easiest to implement and the best established through comparison with experiment. Therefore, they have found the broadest application by workers in the field. The DPM approach has not proven a panacea, however.

The computational shot noise effect, for example, can become intolerable and is especially troubling for such cases as spray combustion instability analyses in which proper assessment of feedback response to local transient flowfield perturbations is an essential element. The shot noise may be reduced by increasing the number of parcels evaluated, which is computationally expensive, or by decreasing the number of computational cells, which reduces the spatial resolution of the analysis. Either alternative incurs a sacrifice.

Accounting for turbulent particle dispersion introduces additional difficulties. An oversimplified DPM approach is the deterministic separated-flow (DSF) model in which the effect of drag due to gas-phase turbulent velocity fluctuations is neglected such that the computational parcels follow deterministic trajectories governed by initial injection conditions and interaction with mean gas flow properties only. Obviously, the DSF model drastically underestimates the transverse spread of the spray. Conversely, the LHF assumption of particle-gas dynamic equilibria overestimates the dispersion rate since slip is neglected. Realistic behavior falls between these two limiting cases, and accurate modeling requires that both parcel and turbulence properties be taken into account. Again, accurate description of particle dispersion is of particular relevance in instability analyses where knowledge of the spray spatial distribution is crucial and oversimplified dispersion models are inappropriate.

Attempts to include turbulent transport for particle dispersion in DPM computations have generally taken one of two forms: 1) introduction of a gradient diffusion expression requiring a turbulent gas-particle exchange coefficient or 2) stochastic separated-flow (SSF) methods based on stochastic simulation of particle motion. The gradient diffusion concept has fallen into disfavor due to the difficulty in obtaining a gas-particle exchange coefficient and the inconvenience of incorporating the model for Lagrangian parcel tracking. The direct modeling SSF methods, on the other hand, have found wider acceptance and show greater promise. These methods entail random sampling for gas-phase turbulent velocity fluctuations based on a specified turbulence model and using the resulting fluctuations in a Lagrangian computation for parcel motion. Most SSF models in practical use are based on variations of the simple ad hoc procedures proposed by Gosman and Ioannides.[5] While advanced techniques that deal directly with Lagrangian correlations of the velocity field from a reference frame on the moving particle eliminate such ad hoc features and yield encouraging results,[6] the conventional SSF models derived from Gosman and Ioannides' approach provide a sufficiently satisfactory description of turbulence-induced dispersion for practical engineering computations. This has been demonstrated for nonevaporating particles through a comparison of computations by Shuen et al.[7] with the fundamental dispersion measurements of Snyder and Lumley[8] in nearly homogeneous, grid-generated turbulence and with the measurements of Yuu et al.[9] in a round, turbulent jet. Evaluation for evaporating droplets in a dilute combusting spray has also been made by Shuen et al.,[10] yielding favorable agreement with experimental results. The computational penalties incurred with these stochastic methodologies are generally heavy, however, since a large number of computational parcels are needed to provide the requisite level of sampling necessary for obtaining a desired level of accuracy in the physical particle distribution profile.

Evidently, the direct modeling approach with turbulent particle dispersion treated as a stochastic process is capable of doing an acceptable job of spray simulation (at least for dilute sprays), but the large number of computational parcels needed to minimize shot noise and produce accurate dispersion distributions can increase computational requirements to unreasonable levels, even for supercomputers. There is, therefore, a real need for more efficient spray modeling techniques. The intent of this paper is to propose one such technique and establish basic validity and improved efficiency through comparison with predictions of the direct modeling SSF methodology for nonevaporating particles injected into a nearly homogeneous turbulent flow and into a round turbulent jet.

## Theoretical Development

The desire is to develop an efficient spray model that will provide a satisfactory representation of turbulent particle dispersion while minimizing random sampling and computational shot noise. Without question, the total number of computational parcels must be limited to meet our primary criterion, efficiency. It also follows that the discrete delta-function characterization for the computational parcels should be relaxed in favor of a distributed representation to meet the desired reduction in shot noise. Furthermore, a simple statistical scheme for evaluating turbulent particle dispersion transport is needed which avoids excessive random sampling without ad hoc simplifications. Constrained by these demands, the conceptual basis for a novel spray combustion modeling technique was formulated.

The fundamental concept of the proposed model is to combine a probability distribution representation for each computational parcel with a statistical turbulent dispersion width transport scheme derived from the direct modeling approach. Specifically, each computational parcel is characterized by a normal (Gaussian) probability density function (pdf) in space. The instantaneous location of each computational parcel, determined from deterministic or stochastic Lagrangian tracking, is taken to represent the mean of its corresponding pdf. In addition, the variance of each pdf, with normalization dependent upon the total number of computational parcels considered, is represented by a statistically derived turbulence-induced mean square dispersion which is dependent upon prior parcel interactions with the characteristic turbulence properties of the flow. The combined pdfs then represent the probable distribution of particles in the spray, including turbulent dispersion effects.

Essentially, this approach merges the statistical distribution aspect of CPMs with the direct modeling approach of DPMs, to obtain the benefits of each without the computational penalties associated with either. For example, letting each computational parcel be represented by a pdf in space alleviates shot noise by distributing interphase source terms over adjoining grid cells and relieves the demand for a high computational-parcel-to-physical-particle ratio. Similarly beneficial, statistical treatment of turbulent particle dispersion based on characteristic parcel–eddy interactions allows for a more generalized approach and reduced sampling. The success of the approach hinges, in fact, on the formulation of just such an efficient procedure for evaluating turbulent particle dispersion transport. In the following section, the basic formulation of this method is presented.

### Dispersion-Width Transport

Development of the transport model for turbulent particle dispersion should begin with a consideration of the fundamental interaction between a particle and an imposed gas-phase velocity field. As such, the fundamental particle equation of motion may be written as

$$\frac{d\boldsymbol{u}_p}{dt} = \frac{3}{4}\frac{\rho_g}{\rho_p}\frac{C_D}{d_p}|\boldsymbol{u}_g - \boldsymbol{u}_p|(\boldsymbol{u}_g - \boldsymbol{u}_p) + \boldsymbol{g} \tag{1}$$

where terms involving negligible effects have been omitted. This first-order ODE is clearly nonlinear and is not analytically integratable. However, if we are willing to sacrifice some accuracy, the equation may be linearized by holding $(\rho_g/\rho_p)(C_D/d_p)|\boldsymbol{u}_g - \boldsymbol{u}_p|$ constant over some small time step. Integration over this time increment results in the expression

$$\boldsymbol{u}_p \approx \boldsymbol{u}_{p0}\exp\left[\frac{-\Delta t}{\tau}\right] + (\boldsymbol{u}_g + \boldsymbol{g}\tau)\left\{1 - \exp\left[\frac{-\Delta t}{\tau}\right]\right\} \tag{2}$$

For a small time increment, the inherent linearization error of this relation is minimized. The relationship for particle displacement is

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p \tag{3}$$

If the linearized particle velocity relationship [Eq. (2)] is introduced into Eq. (3), integration produces a linearized particle displacement equation for a given time increment

$$\Delta\boldsymbol{x}_p \approx \boldsymbol{u}_{p0}\,\tau\left\{1 - \exp\left[\frac{-\Delta t}{\tau}\right]\right\} + (\boldsymbol{u}_g + \boldsymbol{g}\tau)\left[\Delta t - \tau\left\{1 - \exp\left[\frac{-\Delta t}{\tau}\right]\right\}\right] \tag{4}$$

The preceding equations of motion provide for Lagrangian tracking of a particle through the flow. For a nonlinear analysis, Eqs. (1) and (3) may be solved numerically. For a simplified linear analysis, Eqs. (2) and (4) may be utilized by repeated application over a sequence of time steps—the smaller the time step, the more accurate the solution. In a deterministic approach, only the mean gas-phase velocity components are considered. In a stochastic approach, the fluctuating gas-phase velocity components associated with turbulence are included.

It is advantageous at this point, in fact, to re-examine the conventional SSF methodology to solidify the basis for the proposed turbulent transport model. Following the general conception of Gosman and Ioannides,[5] a particle is assumed to interact with a sequence of turbulent eddies, each of which is assumed to have constant turbulence properties. That is, a representative turbulent velocity fluctuation is assumed fully correlated (constant) throughout an eddy's lifetime. The turbulent velocity fluctuation used in each eddy is determined by random sampling over a Gaussian pdf having a mean of zero and a standard deviation corresponding to the root-mean-square (*rms*) turbulent velocity. With the two-equation $k$-$\varepsilon$ turbulence model and the isotropic turbulence assumption, this *rms* turbulent velocity is given by

$$u'_{g_{rms}} = \sqrt{\frac{2k}{3}} \tag{5}$$

An additional elemental assumption is that a particle interacts with an eddy throughout its lifetime or until it traverses the eddy, whichever is shorter:

$$\Delta t_{int} = \min(t_e, t_t) \tag{6}$$

According to Gosman and Ioannides,[5] the characteristic eddy length is assumed to be the dissipation length scale:

$$L_e = \frac{C_\mu^{3/4}\,k^{3/2}}{\varepsilon} \tag{7}$$

For the eddy lifetime, Shuen et al.[7] found the following relation to provide good conformity with experimental observations

$$t_e = \frac{L_e}{u'_{g_{rms}}} = \sqrt{\frac{3}{2}}\frac{kC_\mu^{3/4}}{\varepsilon} \tag{8}$$

A linearized approximation is typically invoked, making use of Eq. (4) and requiring that $|\Delta\boldsymbol{x}_p - \Delta\boldsymbol{x}_{eddy}| = L_e$, to find the transit time

$$t_t = -\tau\,\ln\left[1 - \frac{L_e}{\tau|\boldsymbol{u}_g - \boldsymbol{u}_p|}\right] \tag{9}$$

If $L_e > \tau|\boldsymbol{u}_g - \boldsymbol{u}_p|$ in Eq. (9), the particle is captured by the eddy and will remain trapped until the eddy dissipates.

The described stochastic methodology is known to produce good dispersion results for simple turbulent flows as long as a statistically significant number of particles are considered. It also provides a good conceptual basis for extending fundamental ideas about particle–eddy interactions in developing a scheme for dispersive transport.

Working from the concept of a sequence of particle–eddy interactions, deeper insight may be obtained by recursive application of the linearized equations of motion, Eqs. (2) and (4), with appropriate assumptions. To begin with, mean gas-phase velocity components and gravitational effects are neglected completely since only turbulence-induced dispersion is of interest. Furthermore, letting the linearized equations hold over the entire interaction time, while introducing some error, allows for greater simplification and easier conceptualization. From the standpoint of a transport philosophy, the important implications of such a development are that a turbulence-induced particle velocity within a particular eddy propagates to affect all subsequent interactions and that this transport of turbulence-induced dispersion may be expressed entirely in terms of turbulence strength, particle–eddy interaction time, and the particle inertial time lag.

Therefore, if one wishes to express the turbulence-induced displacement after the $n$th eddy interaction, a combination of relations describing previous influential interactions is required. Of course, the cascading effects of early interactions can have an increasingly minor affect on later interactions downstream, so that it may not be necessary to carry this influence beyond some arbitrary number of eddies. Such subtle particularities are not known a priori, however, and it is wise to begin with the most general expression in which each interaction history is transported through all subsequent interactions up to the $n$th eddy.

Following this approach, the linearized particle velocity equation is evaluated for an initial interaction considering turbulence effects only. This result may then be substituted into the evaluation for the following interaction. Repeated substitution and evaluation for every subsequent interaction yields a single expression for $u_p'$ after the $n$th eddy interaction which contains the entire particle history as influenced by turbulence:

$$u'_{p_n} \approx \sum_{i=1}^{n-1} u'_{gi}\left\{1-\exp\left[\frac{-\Delta t_i}{\tau_i}\right]\right\} \times \begin{bmatrix} \exp\left[-\sum_{j=i+1}^{n-1}\left(\frac{\Delta t_j}{\tau_j}\right)\right]; & i<n-1 \\ 1 & ; i=n-1 \end{bmatrix} \tag{10}$$

The bracketed terms on the RHS represent the manner in which a turbulent velocity fluctuation in the $i$th eddy acts through subsequent interactions to influence the turbulence-induced particle velocity after the $n$th eddy.

Similar evaluation for the linearized particle displacement equation yields an expression for the dispersive displacement after the $n$th eddy interaction:

$$\Delta x'_{pn} \approx \sum_{k=1}^{n} u'_{gk}\left[\Delta t_k - \tau_k\left\{1-\exp\left[\frac{-\Delta t_k}{\tau_k}\right]\right\}\right] + \sum_{k=1}^{n} u'_{pk}\tau_k\left\{1-\exp\left[\frac{-\Delta t_k}{\tau_k}\right]\right\} \tag{11}$$

A relation for turbulent dispersion is our aim, but we desire to have the expression completely in terms of the gas-phase turbulent velocity fluctuations, the interaction times, and the particle relaxation times. Since Eq. (11) contains $u'_{pk}$, which carries the history of previous interactions, it is advantageous to substitute Eq. (10) to obtain a relation of the form

$$\Delta x'_{pn} \approx \sum_{k=1}^{n} u'_{gk}\, T_k \tag{12}$$

where $T_k$ is essentially an effective time constant for turbulent dispersion which accounts for the influence of the $k$th interaction on dispersion at the $n$th eddy. Making the substitution and the necessary manipulations produces the desired form where $T_k$ is given by

$$T_k = (\Delta t_k - \tau_k A_k) + \begin{Bmatrix} A_k \sum_{i=k+1}^{n} \begin{Bmatrix} \tau_i A_i \exp\left[-\sum_{j=k+1}^{i-1}\left(\frac{\Delta t_j}{\tau_j}\right)\right]; & i>k+1 \\ \tau_i A_i & ; i=k+1 \end{Bmatrix}; & k<n \\ 0 & ; k=n \end{Bmatrix} \tag{13}$$

with $A_l$ defined as

$$A_l = \left\{1-\exp\left[\frac{-\Delta t_l}{\tau_l}\right]\right\} \tag{14}$$

Note that $T_k$ is dependent on the $n$th eddy under consideration due to the recursive nature of the formulation where $T_k$ is evaluated for the eddies $k \rightarrow n$. It should be possible to truncate the number of interaction evaluations for $T_k$ as the influence of the $k$th eddy decays so that only eddies $k \rightarrow m$ need be considered where $m \le n$. Such improvements in efficiency are of practical importance, but a critical analysis of the truncation criteria is left to future study.

Essentially, Eq. (12) is a simplified linearization of the SSF model. Here, under the presupposition of particle/parcel dynamic duality, the dispersion for each computational parcel after the $n$th eddy interaction is compacted within a single recursive expression. Evaluation for a statistically significant number of parcels should be expected to produce a reasonable approximation of the physical particle distribution profile downstream from injection. Our purpose, however, is to obtain a generalized description for turbulent dispersion transport and avoid such excessive sampling.

This generalization is made possible from statistical inferences concerning particle–eddy interactions and the implications from Eq. (12) which follows. For instance, we first note that the turbulent gas-phase velocity fluctuations are considered fully correlated (constant) within each eddy and that there is no cross-correlation between eddies. Then Eq. (12) represents a linear combination of $n$ mutually independent random variables, $u'_{gk}$. If we further recognize that $u'_{grmsk}$ represents the standard deviation for each random variable $u'_{gk}$, we can then form the variance for the linear combination of random velocity fluctuations implied by Eq. (12) as a sum of squares characterizing the dispersion width

$$\sigma^2_{pn} \approx \sum_{k=1}^{n} (u'_{grmsk}\, T_k)^2 \tag{15}$$

where $\sigma^2_{pn}$ is the overall mean square dispersion corresponding to the variance of the parcel pdf after the $n$th interaction.

This is the fundamental statistical relation sought for turbulent particle dispersion transport. To apply Eq. (15), a parcel is directly tracked (either deterministically or stochastically) through a sequence of eddies to determine its mean position while evlauating $u'_{grms}$, $t_{int}$, and $\tau$ for each interaction. These turbulence properties may then be used to calculate the variance of the computational parcel's pdf after each interaction. In this paper, two models are proposed to calculate the mean positions of the computational parcels. Both models employ Lagrangian tracking. For tracking in which the gas-phase turbulent velocity fluctuations are neglected, the approach is described as a deterministic dispersion-width transport (DDWT) model. In this case, $\tau$ should be evaluated by using characteristic turbulent velocity fluctuations (e.g., the *rms* values) to determine a characteristic relative velocity for each interaction. With tracking based on random sampling over the gas-phase turbulent velocity pdf, the approach is described as a stochastic dispersion-width transport (SDWT) model. When convoluting pdfs associated with an ensemble of computational parcels, the variances of Eq. (15) must be normalized according to the total number of parcels being combined. This issue is addressed in the following section.

#### Convolution of PDFs

Because practical turbulent flows within spray combustors are complex and invariably inhomogeneous, multiple parcel ensembles will be necessary to simulate the spray. Since this requires convolution of the computational parcel pdfs, it follows that the variance computed for each pdf should be normalized by the total number of computational parcels associated with a given ensemble to obtain the proper dispersion width. This normalization is written here in the form

$$\hat{\sigma}_{r_i} = K \frac{\sigma_{r_i}}{\sqrt{N_{cp}^{(e)}}} \tag{16}$$

where $\sigma_{r_i}/\sqrt{N_{cp}^{(e)}}$ represents the statistical uncertainty in the mean parcel position and $K$ is introduced as a correction factor to account for undersampling. As $N_{cp}^{(e)} \to N_{pp}^{(e)}$ we impose $\hat{\sigma}_{r_i} \to 0$ such that the discrete delta-function SSF model is recovered.

In general, parcel ensembles will be formed from physical particles sharing a common injection time. These physical particles are grouped to form a particular total parcel number which satisfies a desired parcel-to-particle ratio. Each particle group will then remain associated with a specific parcel throughout its life history. When evaluating for an ensemble containing a single parcel, $K = 1$ and $\hat{\sigma}_{r_i} = \sigma_{r_i}$.

#### Axisymmetric Parcel PDF

Since in general each computational parcel is represented as a three-dimensional normal pdf, integration over three spatial coordinates is required to determine the probability of locating a physical particle at a given position. This integration may be simplified for the special case of axial symmetry where turbulent velocity fluctuations in the axial direction are relatively weak with respect to transverse velocity fluctuations which corresponds to the round turbulent jet test problem of specific interest in this paper. By neglecting the mild dispersive effect in the predominant flow direction, integration over the normal pdf is required only in planes perpendicular to the symmetry axis. Statistically, this implies $\sigma_{ax} \to 0$ for the axial coordinate.

To perform the integration, consider the normal, single-coordinate pdf in a plane parallel to and intersecting the axis of symmetry with a mean $r_p$ and a standard deviation $\sigma_r$ as shown in Fig. 1. Then a cumulative distribution at any coordinate $r$ may be defined as the volume swept out by the pdf bounded by $-r \le R \le r$ as it is revolved 360 deg about the axis of symmetry. After integration the axisymmetric cumulative distribution function takes the form

$$\begin{aligned} F(r) = \sqrt{2\pi}\sigma_r \Bigg[ 2\exp\left[-\frac{1}{2}\left(\frac{r_p}{\sigma_r}\right)^2\right] \\ - \exp\left[-\frac{1}{2}\left(\frac{r-r_p}{\sigma_r}\right)^2\right] - \exp\left[-\frac{1}{2}\left(\frac{r+r_p}{\sigma_r}\right)^2\right]\Bigg] \\ + 2\pi r_p \Bigg[\left\{\Phi\left(\frac{r-r_p}{\sigma_r}\right) - \Phi\left(\frac{-r_p}{\sigma_r}\right)\right\} \\ - \left\{\Phi\left(\frac{r+r_p}{\sigma_r}\right) - \Phi\left(\frac{r_p}{\sigma_r}\right)\right\}\Bigg] \end{aligned} \tag{17}$$

where

$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left[\frac{-Z^2}{2}\right] dZ \tag{18}$$

which is the cumulative distribution function of a single-coordinate standardized normal random variable readily available from tabulations or computations by standard algorithms.

By definition, a cumulative distribution function should approach unity as the argument approaches infinity. To ensure this condition for the axisymmetric case, we should normalize by $F(r \to \infty)$ given by

$$\begin{aligned} F(r \to \infty) = 2\sqrt{2\pi}\sigma_r \exp\left[-\frac{1}{2}\left(\frac{r_p}{\sigma_r}\right)^2\right] \\ + 2\pi r_p \left[\Phi\left(\frac{r_p}{\sigma_r}\right) - \Phi\left(\frac{-r_p}{\sigma_r}\right)\right] \end{aligned} \tag{19}$$

It is then possible to define the probability that a random variable will be less than or equal to the radius $r$ as

$$P(r) = \frac{F(r)}{F(r \to \infty)} \tag{20}$$

which is the axisymmetric probability relation desired.

To describe the time-averaged dispersion for a dilute spray where particle loading effects are negligible, it is sufficient to combine all parcels into a single ensemble independent of injection time. Convolution of the probability distributions for every parcel in such an ensemble at a designated cross section of the flow yields the time-averaged probable physical particle distribution.

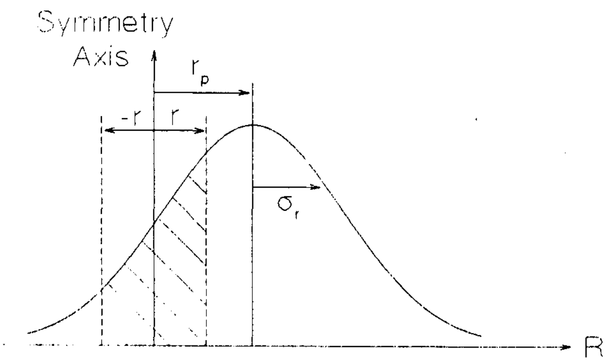


**Fig. 1 Schematic of single-coordinate normal pdf in a plane parallel to and intersecting the axis of symmetry.**

## Results

Evaluation of the proposed dispersion-width transport model was made by comparison with the delta-function SSF model, which has been well verified for simple turbulent flows. Specifically, time-averaged dispersion computations were made for nonevaporating particles injected into a nearly homogeneous turbulent flow of air and into a round turbulent air jet. A time-dependent evaluation for ensembles having parcels grouped according to a common injection time is left to future study. Particle sizes and densities were chosen to obtain a wide range in values for the particle relaxation times. By judicious selection, cases could be examined in which the eddy lifetime controls interaction times, the transit time controls interaction times, or the interaction times undergo transition from control by the transit time to control by the eddy lifetime.

#### Dispersion in Nearly Homogeneous Turbulence

The empirically described grid-generated turbulence from Snyder and Lumley's experimental work[8] was applied as a simple representative natural turbulent flow. Measurements indicated homogeneous turbulence in planes transverse to the flow and mild inhomogeneity with the flow due to turbulence decay. The turbulence was also found to be very nearly isotropic. Empirically derived analytic equations were presented for the turbulent kinetic energy as a function of axial position from which the dissipation is obtainable by differentiation. With the mean velocity and turbulent kinetic energy and dissipation known throughout the flow, dispersion computations could be made.

For the delta-function SSF computations, single particles were repetitively injected into the flow 20 mesh lengths from the grid. Due to low particle loading, interphase momentum coupling was neglected. Dispersion from the centerline was stored at designated cross sections and times for each particle. After evaluating the desired numer of particles, a mean square dispersion was calculated with reference to a specified axial position or time following injection. For the DDWT computations, a single parcel was evaluated following a deterministic trajectory along the centerline. With the necessary parameters for each interaction, the mean square dispersion was computed from Eq. (15) representing the variance of the parcel pdf.

Shown in Fig. 2 are the resulting mean square dispersion and characteristic particle relaxation time constants with respect to axial distance from injection with no initial slip ($u_{p0} = \overline{u_g} = 6.55$ m/s). The DDWT model, using a single computational parcel, shows good agreement with the delta-function SSF predictions using 5000 particles for a wide range in particle mass. Examination of the characteristic particle relaxation time constants for each parcel–eddy interaction reveals the various controlling interaction times considered. Similarly good agreement for the mean square dispersion is shown in Fig. 3 when significant initial slip ($u_{p0} = 1$ m/s) is introduced. The characteristic particle relaxation time constants for this initial slip case reveals the delayed response of the heavier particles to the initial relative mean velocity difference and the almost instantaneous attainment of the mean gas-phase velocity by the lightest particle. Comparable agreement for dispersion was also obtained with respect to time from injection.

In Figs. 2 and 3, a certain waviness in the mean square dispersion curve was produced by the delta-function SSF model for the lightest particle considered. This behavior may appear anomalous but is really an anticipatory mathematical result of the SSF model. Because the turbulence is essentially homogeneous throughout this uniform flow, the SSF model implies that all particles will basically see the same sequence of turbulent eddy time and length scales regardless of the individual stochastic trajectories. Furthermore, light particles associated with sufficiently small time constants will equilibrate quickly with any velocity fluctuation so that the interaction time scale will be governed by the eddy lifetime. This behavior is clearly demonstrated by the lightest particle in Figs. 2 and 3. Therefore, each wave in the concerned curves represents the combined effect of every particle in the sample equilibrating with a turbulent eddy velocity fluctuation through an exponential-like decay function. This argument is additionally supported by the observation that each wave is associated with a particular data point of the DDWT model where every such data point corresponds to a particular eddy.

Since the delta-function SSF model produced Gaussian particle distributions, it follows that the normal pdf parcel characterization of the DDWT model provides an identical description. With a single computational parcel following a deterministic trajectory, the dispersion width transport model demonstrates the capability of producing accurate time-averaged dispersion results with minimal computational requirements for this simple turbulent flow. That a single sample of the particle–eddy interactions is sufficient to describe dispersion in this flow is of no great distinction, however, since the turbulence is homogeneous in the transverse plane and additional sampling would contribute negligible perturbations.

#### Dispersion in a Round Turbulent Jet

A more stringent test case is for particles injected into a round turbulent air jet where the turbulence is inherently inhomogeneous. The PDEs for steady axisymmetric boundary-layer flow are solved using a modified version of the well-known GENMIX code with a $k - \varepsilon$ turbulence model. The jet is directed upward against the gravitational force. The nozzle diameter was 2.18 cm with a mean exit velocity of 26 m/s. Particles were ejected at the mean nozzle exit velocity, and particle loading effects were neglected.

To demonstrate the effect of inhomogeneity, comparison of predicted mean square dispersion by the delta-function SSF model using 8000 particles and the DDWT model using a single parcel is shown in Fig. 4 along with the characteristic particle relaxation time constants. Agreement for the heavy particle is good since there is little deviation from the centerline. Sampling with a single parcel along the centerline is therefore adequate. For the lighter particles, however, deviation is significant and centerline particle–eddy interaction properties are inadequate to describe dispersion for the jet flow. Additional sampling of particle–eddy interactions away from the injection axis is required.

Introduction of the stochastic approach for determining computational parcel trajectories (SDWT model) is therefore needed. For illustrative purposes, examination is made for particles with the properties $d_p = 50$ μm and $\rho_p = 1000$ kg/m$^3$ injected into the jet which has been divided into 30 concentric equal radius cells at each cross section of interest. First, calculations using the nonlinear delta-function SSF model were

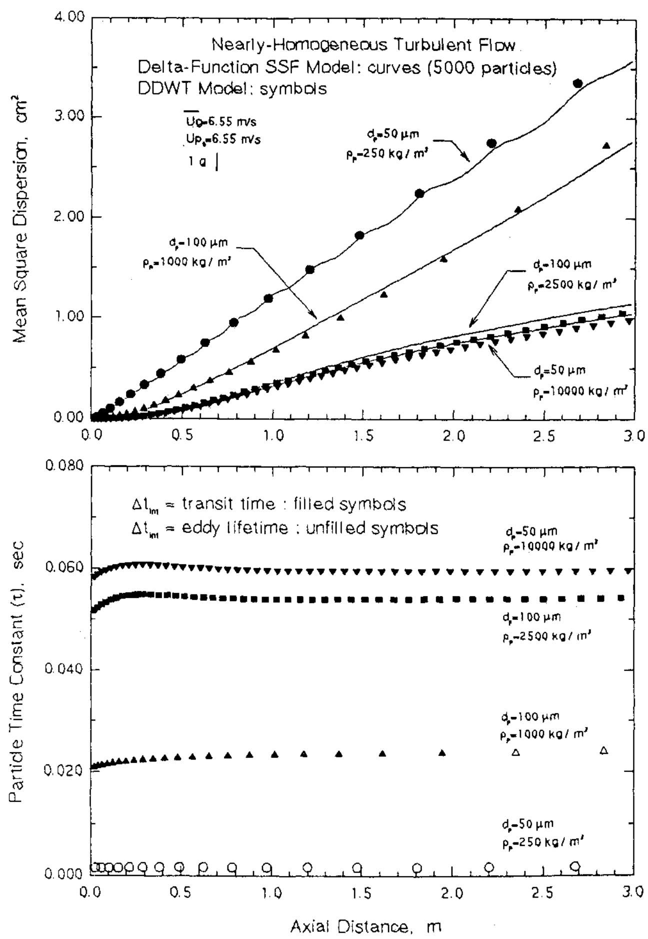


**Fig. 2 Mean square dispersion and characteristic particle relaxation time constants with respect to axial position for particles injected into a nearly homogeneous flow (no initial slip).**

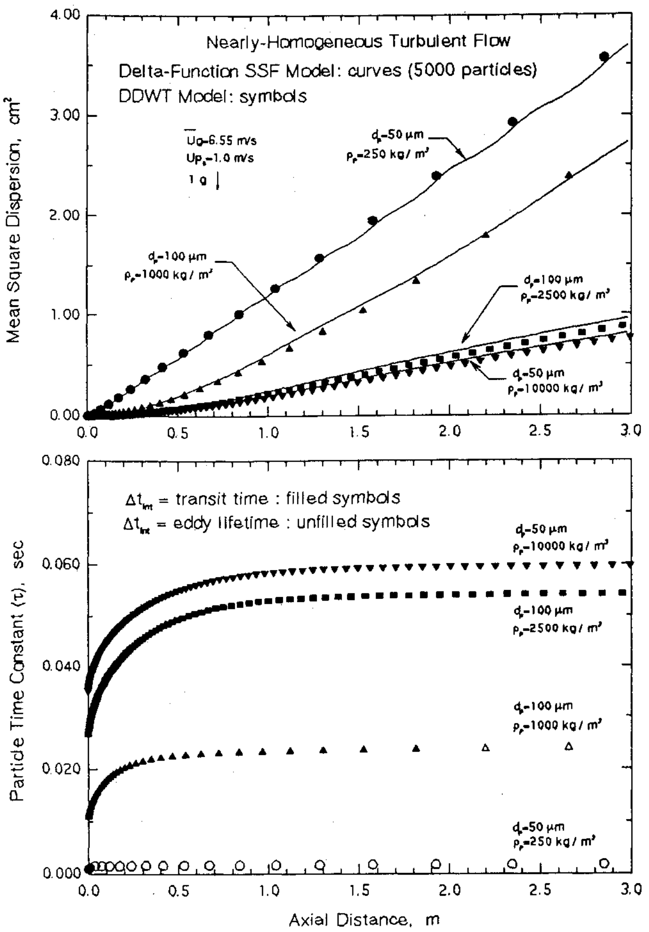


Fig. 3 Mean square dispersion and characteristic particle relaxation time constants with respect to axial position for particles injected into a nearly homogeneous flow (with initial slip).

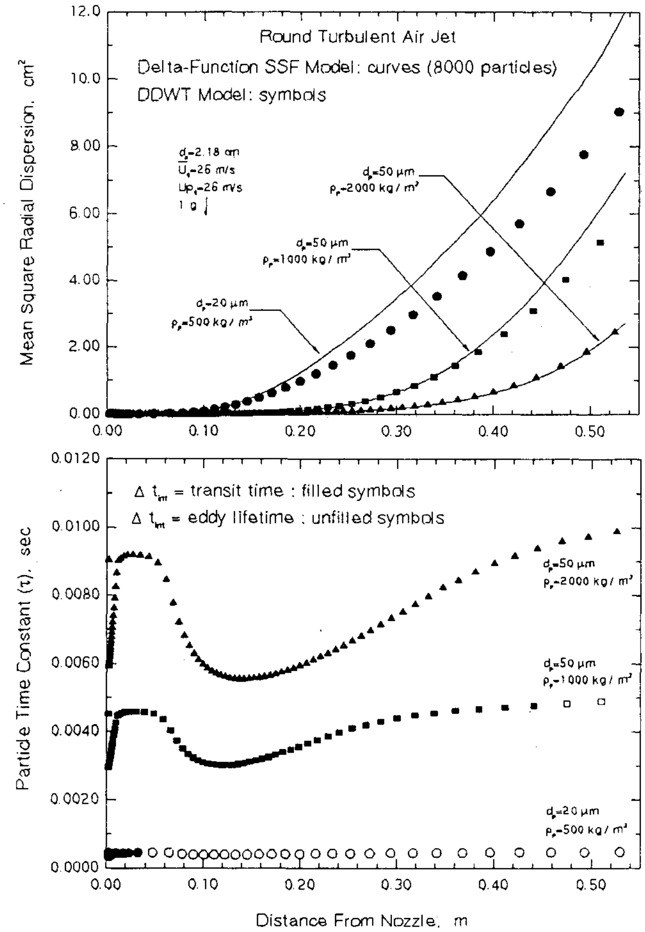


Fig. 4 Mean square dispersion and characteristic particle relaxation time constants with respect to axial position for particles injected into a round turbulent jet.

made for a baseline comparison. Figure 5 shows the time-averaged probable physical particle fraction per cell obtained at three axial locations using a 20,000-particle sample as well as a comparison of results based on 50-, 500-, and 20,000-particle samples at $x/d_n$ = 24.58. For the 20,000-particle case there is some evidence of slight undersampling, but the distribution is statistically stationary and is taken as a fair theoretical representation of the time-averaged results one might obtain in an actual physical experiment. Note that the profiles collapse to a characteristic distribution independent of distance from the nozzle when the radial coordinate is reduced by the standard deviation. Also observe that the profiles for the 50- and 500-particle cases are very irregular and unsuitable. On a brief note, these figures may be disconcerting to some readers because they exhibit off-axis maxima; however, they should not be construed as concentration profiles. If the particle fraction for each cell were normalized by the corresponding cell volume, concentration profiles would be obtained exhibiting the expected on-axis maxima.

Computations with the SDWT model at $x/d_n$ = 24.58 using various values for the correction factor are shown in Fig. 6 for a 50-parcel ensemble. This 50-parcel case is somewhat sensitive to the value of the correction factor as expected since the spray is grossly undersampled. By increasing $K$ above unity, however, correction for uncertainty in the mean increases the dispersion and smooths the profile considerably. It should be noted here that the distribution obtained with the SDWT model is sensitive to the random numbers generated for sampling the gas-phase turbulent velocity fluctuation pdf, and the use of the correction factor $K$ helps alleviate any skewness and irregularity due to undersampling. A correction factor of $K \approx 2$ is found optimal for approximating the theoretical distribution in this flow.

The time-averaged physical particle pdfs as determined from the delta-function SSF and SDWT models are now compared at three axial locations in Fig. 7. With only 50 parcels, the SDWT model produces smooth and relatively accurate distributions which are even better than the delta-function SSF model using 500 particles. Dispersion is well described by the SDWT model throughout the jet length. The SDWT model seems clearly capable of describing dispersion in inhomogeneous turbulent flows with improved efficiency over the delta-function SSF model.

## Concluding Remarks

The formulated statisical transport model for turbulent particle dispersion has been shown to provide a good approximation of time-averaged dispersion in comparison to the conventional delta-function SSF model, for nonevaporating particles in nearly homogeneous turbulence and in a round turbulent jet. For turbulence that is homogeneous in transverse planes of a uniform flow, the DDWT model was found to sample sufficiently the particle–eddy interactions using a single computational parcel such that accurate dispersion profiles are obtained. For the round turbulent jet, additional sampling using the SDWT model was required due to inhomogeneity in the turbulence. The required sampling in this case was still significantly lower than required for the conventional SSF approach.

Principle implications of the proposed model include the potential for significantly improving the computational effi-

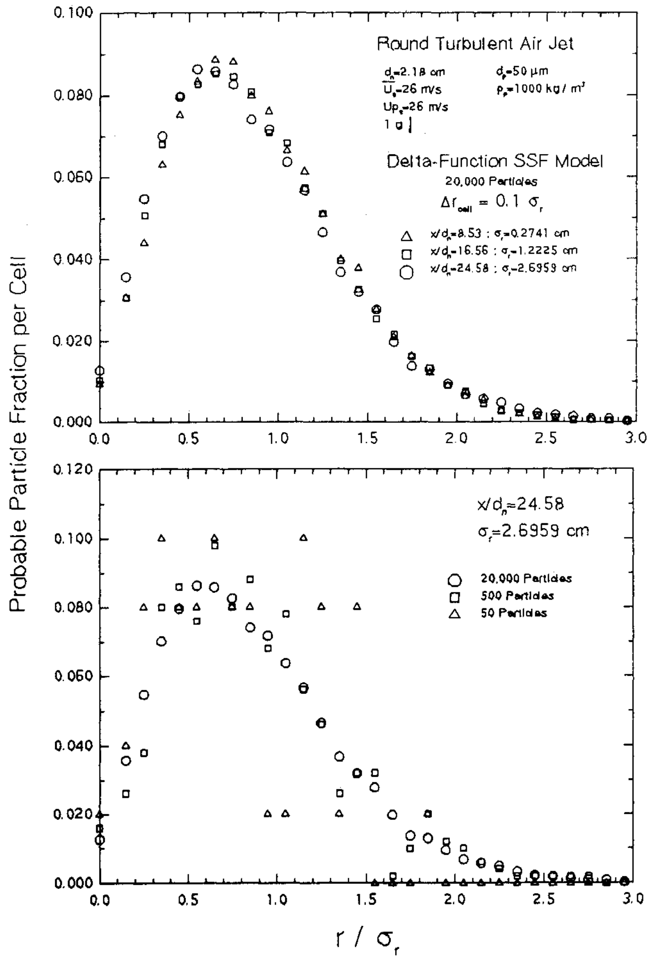


**Fig. 5 Time-averaged probable physical particle fraction per cell for a round turbulent jet according to delta-function SSF model.**

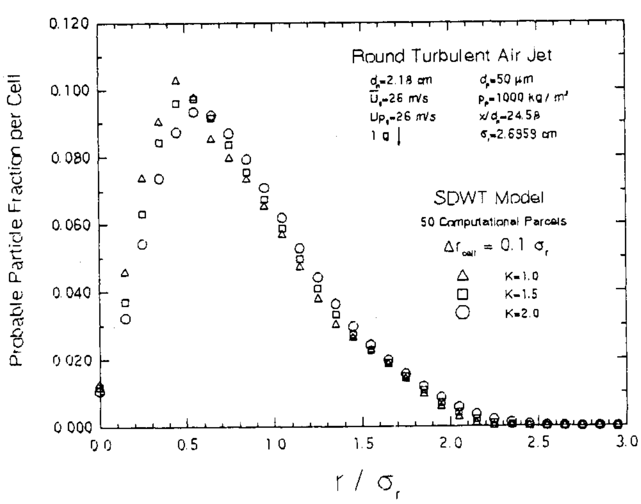


**Fig. 6 Time-averaged probable physical particle fraction per cell for a round turbulent jet according to SDWT model using 50 computational parcels with various correction factor values.**

ciency of spray combustion CFD analyses and for minimal production of computational shot noise. Gains in efficiency should follow from the use of a lower ratio of parcel number to particle number. Although the proposed model requires the additional computation of a variance for each parcel pdf, the operation count will still be lower than that of the delta-function SSF model for some slightly larger parcel-number-to-particle-number ratio. Along these lines, additional efficiency should be obtainable with the model by limiting the

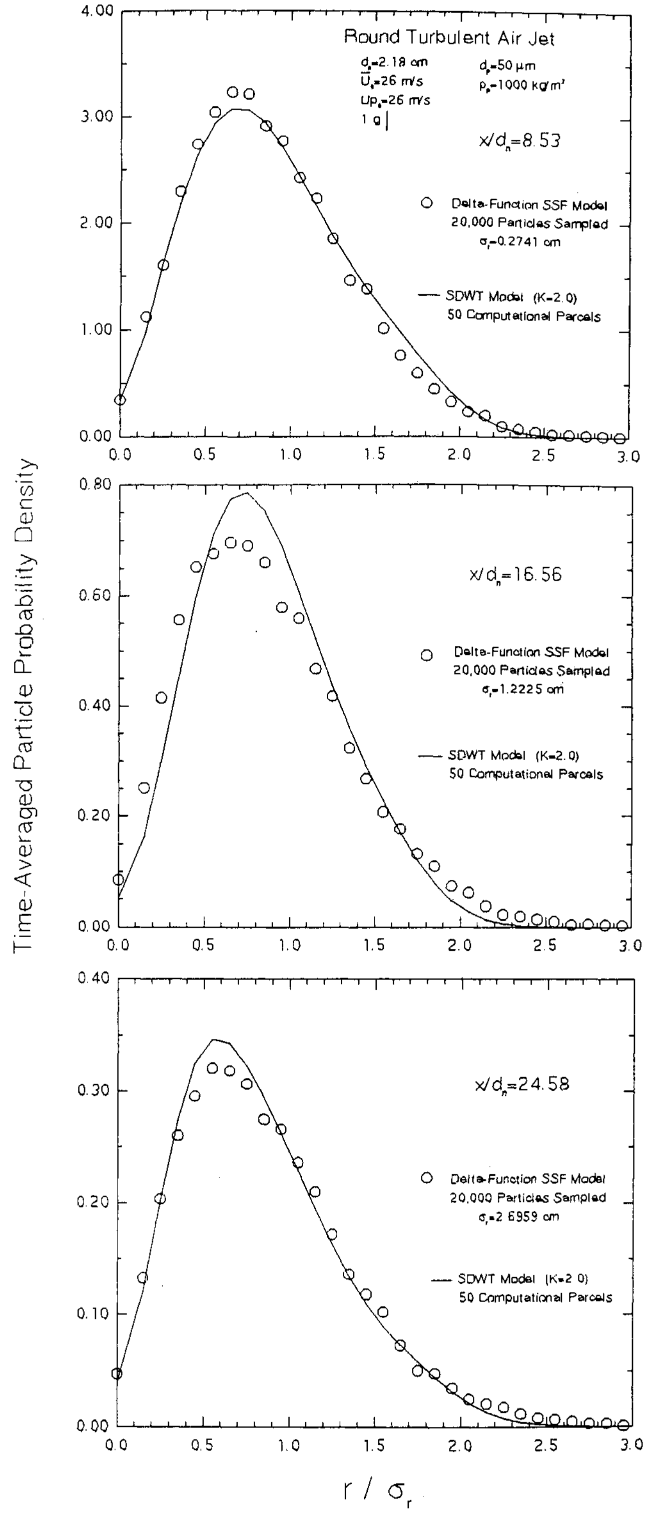


**Fig. 7 Time-averaged physical particle pdf at three axial locations of a round turbulent jet according to delta-function SSF and SDWT models.**

influence of a turbulence-induced particle velocity within a particular eddy to subsequent interactions in which it makes a non-negligible contribution. This will allow truncation of unnecessary computations in the evaluation of the parcel pdf variance. Minimal shot noise production will follow from the statistical distribution representation for each parcel, which will allow for a more continuous distribution of interphase transport sources. Therefore, the proposed dispersion-width transport model holds high promise for improving the accuracy and efficiency of spray combustion CFD codes.

Planned future development of the approach will involve evaluation for a dilute evaporating droplet spray followed by extension to more complicated flows representative of practical spray combustors where the flow is heavily laden with droplets. Practical implementation will demand that time dependence be considered where parcel ensembles are formed from particles sharing a common injection time and that efficient distribution of interphase transport sources be addressed. Concerning this matter, it will be beneficial to investigate alternative pdfs such as a uniform distribution to obtain greater simplicity. Evaluation using alternative turbulence models would also be desirable.

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